


## Curriculum vitae – Carlo Gatti

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<b>Full name</b>	Carlo Gatti
<b>Personal Details</b>	Born 4 December 1954; married to Alessandra Silvani Three children: Elena (40), Francesco (25) and Emanuela (23)
<b>Address</b>	CNR-SCITEC (Istituto di Scienze e Tecnologie Chimiche Giulio Natta, sezione di via Golgi) c/o Dept. Of Chemistry, Università degli Studi di Milano, via Golgi 19, 20133 Milano (Italy)
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<b>Academic Qualifications</b>	Dr (1978), Chemistry and Theoretical Physical Chemistry, Univ. of Milano

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## Habilitations/Qualifications

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- **2020** January Habilitation ("Abilitazione Scientifica Nazionale, tornata 2018-2020") as **University full professor** for the following disciplines ("settori concorsuali"): a) 03/A2 Modelli e Metodologie per le Scienze Chimiche (Physical Chemistry); b) 03/B2 Fondamenti Chimici delle Tecnologie (Chemistry for Engineering Science)
- **2019**, 24 December : **Dirigente di ricerca CNR**, first position, "secondo scorrimento", bando 367.161; 2 March 2020 permanently hired as **Dirigente di ricerca CNR**
- **2019** December Habilitation ("Abilitazione Scientifica Nazionale, tornata 2018-2020") as **University full professor** for the following discipline ("settor concorsuale"): 03/B1 Fondamenti delle Scienze Chimiche e Sistemi Inorganici (Inorganic Chemistry)
- **2018** Habilitation ("idoneo") as "Dirigente di Ricerca CNR" (8th placement, Competition for the "profilo professionale Dirigente di Ricerca-I Livello- Area Strategica Materiali Innovativi, tecniche Avanzate di caratterizzazione e modelling, bando n. 367.161
- **2016**: 24/6/2016, Habilitation ("idoneo") as "Dirigente di Ricerca CNR" (27th placement, Competition for the "profilo professionale Dirigente di Ricerca-I Livello- area disciplinare Scienze Chimiche, bando n. 364.172).
- **2015** Habilitation ("Abilitazione Scientifica Nazionale", "tornata 2013") as **University full professor** for the following disciplines ("settori concorsuali") : a) 03/A2 Modelli e Metodologie per le Scienze Chimiche (Physical Chemistry); b) 03/B2 Fondamenti Chimici delle Tecnologie (Chemistry for Engineering Science)
- **2014** Habilitation ("Abilitazione Scientifica Nazionale", "tornata 2012") as **University full professor** for the following disciplines ("settori concorsuali") : a) 03/A2 Modelli e Metodologie per le Scienze Chimiche (Physical Chemistry); b) 03/B1 Fondamenti delle Scienze Chimiche e Sistemi Inorganici (Inorganic Chemistry); c) 03/B2 Fondamenti Chimici delle Tecnologie (Chemistry for Engineering Science)
- **2011**: 17/2/2011 Habilitation ("idoneo") as "Dirigente di Ricerca CNR" (10th placement, Competition for the "profilo professionale Dirigente di Ricerca-I Livello- area disciplinare Scienze Chimiche, bando n. 364.86)
- **2006**: 19/7/2006 Habilitation ("idoneo") as "Dirigente di Ricerca CNR" (42th placement, Competition for the "profilo professionale Dirigente di Ricerca-I Livello- area disciplinare Scienze Chimiche, bando n. 364.7).

## Professional/Academic Experience

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| <b>1979-1982</b>   | Research contracts with industries and national energy agencies for the reduction of radioactive contamination in nuclear plants |
| <b>1982-1986</b>   | "Collaboratore Tecnico Professionale" CNR, CNR-CSRSRC (Milano)   |
| <b>1986-1999</b>   | CNR Research Scientist, CNR-CSRSRC (Milano)  |
| <b>1999-2019</b>   | CNR Senior Research Scientist, at CNR-CSRSRC and then at CNR-ISTM (Milano) and now at CNR-SCITEC                                 |
| <b>2019 Dec 24</b> | Dirigente di ricerca CNR (prima posizione secondo scorrimento concorso 367.161), assunto in data 2 marzo 2020                    |
| <b>1986-1989</b>   | Visiting scientist McMaster Univ.(Prof. RFW BADER's lab), Hamilton (Ontario), Canada for a total of 6 months                     |

- 1992 Visiting scientist IVIC, Caracas, Venezuela, for 2 months (Prof. Juan Murgich)
- 1996-1997 Visiting scientist, Center of Crystallographic Studies (Prof. Sine Larsen), Copenhagen, Denmark for about 2 weeks
- 1999 Visiting scientist Department of Chemistry (Prof. Finn Larsen), University of Aarhus, DK (one week)
- 1999-2000 Visiting scientist, Dept. of Chemistry (Prof. P. Coppens), SUNY Buffalo, USA, for a total of one month
- 2007 Visiting scientist LCM3B, (Prof. Claude Lecomte), Nancy, France, for one month
- 2009 Visiting scientist Institut für Organische Chemie (Prof. Bernd Engels), Universität Würzburg, Germany, for one week
- 2014 Visiting scientist LRCS-CNRS ([Réactivité et Chimie des Solides](#)), UMR 7314 (Prof. C. Frayret) Université Jules Verne, Amiens (France) for one month
- 2015 Professor of PhD course, 'École Doctorale Sciences, Technologie, Santé – EDSTS, and visiting scientist at LRCS-CNRS ([Réactivité et Chimie des Solides](#)), UMR 7314 ((Prof. C. Frayret), Université Jules Verne, Amiens (France) for one month
- 2017 Visiting scientist LRCS-CNRS ([Réactivité et Chimie des Solides](#)), UMR 7314 (Prof. C. Frayret) Université Jules Verne, Amiens (France) for one month
- 2017 Visiting scientist Department of Physics (Prof. M. Wüttig), RWTH Aachen University, Germany, Lab. (four short visits for a total of seven working days)
- 2018 Professor of PhD course, 'École Doctorale Sciences, Technologie, Santé – EDSTS, and visiting scientist at LRCS-CNRS ([Réactivité et Chimie des Solides](#)), UMR 7314 ((Prof. C. Frayret), Université Jules Verne, Amiens (France) for three weeks
- 2018 Visiting scientist Department of Physics (Prof. M. Wüttig), RWTH Aachen University, Germany, Lab. (two short visits for a total of five working days)
- 2019 Visiting scientist LRCS-CNRS ([Réactivité et Chimie des Solides](#)), UMR 7314 (Prof. C. Frayret) Université Jules Verne, Amiens (France) for three weeks
- 2019 Visiting scientist Department of Physics (Prof. M. Wüttig), RWTH Aachen University, Germany, Lab. (two short visits for a total of six working days)
- 2020 Visiting scientist LRCS-CNRS ([Réactivité et Chimie des Solides](#)), UMR 7314 (Prof. C. Frayret) Université Jules Verne, Amiens (France) for three weeks, application approved, but the visits to the Jules Verne University have been delayed because of the COVID affair.
- 2021-2022 Visiting scientist LRCS-CNRS ([Réactivité et Chimie des Solides](#)), UMR 7314 (Prof. C. Frayret) Université Jules Verne, Amiens (France) for three weeks, application approved

2010-2022 Carlo Gatti is one of the six international partners of the Center for Materials Crystallography (CMC, <http://cmc.chem.au.dk/>), a new Centre of Excellence established January 1st, 2010, based on funding from The Danish National Research Foundation. The Center is headed by Prof. Bo Bummerstedt Iversen (Aarhus University, DK) and the six international partners are:

- Prof. Dr. Dietmar Stalke (Georg-August-Universität Göttingen, Germany)
- Prof. Mark Spackman (University of Western Australia, Australia)
- Dr. **Carlo Gatti** (Istituto di Scienze e Tecnologie Molecolari, Italy)
- Research Director Masaki Takata (SPring8 Synchrotron Facility, Japan)
- Exec. Director P. James Viccaro (University of Chicago Center for Advanced Radiation Sources, USA)
- Group Leader Bryan Chakoumakos (Neutron Scattering Division, Oak Ridge National Laboratory, USA)

The CMC is aimed at exploiting the revolutionising opportunities provided by new X-ray and neutron sources to tackle important challenges in materials science. These include:

- Unraveling the chemical origin of molecular self-assembly
- Understanding the mechanism behind thermoelectric materials capable of converting heat into electrical energy,
- Measuring structures of laser excited crystals
- Understanding the nucleation, growth and structure of the nanoparticles, which form the basis of emerging new energy technologies
- Quantifying how guest molecules interact with porous host materials used e.g. for gas storage or catalysis
- Obtaining an atomic scale insight into complex magnetic materials

The expertise and contribution of Dr Gatti within CMC concerns the ab-initio calculations of periodic systems, the development of new software implementing quantum topological approaches (such as Quantum Theory of Atoms in Molecules, QTAIM, Bader's theory) for the

solid state and of new chemical bond descriptors, in particular the source function.

## Leadership

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2000-2021	Member of the Scientific Board or of the International Advisory Board of numerous congresses during past 20 years
2018	Chair of the International Miguel Blanco Prize 2018 Selection Committee, <a href="http://www.sagamore2018.ca/m-blanco-international-prize/">http://www.sagamore2018.ca/m-blanco-international-prize/</a>
2017	Chair of the Round Table on <i>Future Perspectives and a Vision for Quantum Crystallography</i> , CECAM meeting CECAM Discussion Meeting on Quantum Crystallography: Current Developments and Future Perspectives, Nancy, 19-20 June 2017
2016	Conference chair, along with Prof. Artem Oganov and Dr. Davide Ceresoli of the International Symposium on Material Design & the 11 <sup>th</sup> USPEX workshop, villa Monastero, Varenna, Lake Como, Italy, 5-9 June 2016
2015	Conference Chair of Sagamore XVIII meeting (on Charge Spin and Momentum Densities (S. Margherita di Pula, Cagliari, Italy) 7-12 June 2015).
2011 up to now	Consultant of the International Union of Crystallography (IUCr) Commission on Charge Spin and Momentum Densities (since August 2017 with the new name for this Commission, i.e. IUCr Commission of Quantum Crystallography)
2008-2011	<b>Chair</b> of the International Union of Crystallography (IUCr) Commission on Charge Spin and Momentum Densities. Appointed to this IUCr Commission in 1999, and served three consecutive three-years terms. Elected to Chair this Commission for the period 2008-2011 at the Osaka 2008 IUCr Congress. The Commission's aim is to promote the broad field of experimental and theoretical determinations and analysis of charge, spin and momentum distributions, and it does this by the organization of conferences, workshops, and the overseeing of international projects with well-defined objectives
1999-2008	Member of the International Union of Crystallography (IUCr) Commission on Charge Spin and Momentum Densities
1999-2011	Member and Secretary of the European Crystallographic Association (ECA) Special Interest Group (SIG) on Charge Spin and Momentum Densities (CSMD, SIG-2) since 1999 up to 2011
2005-2010	Served for three times (2005-2006, 2007-2008, 2009-2010) as a official <b>international reviewer of the DFG</b> (Deutsche Forschungsgemeinschaft) priority program SPP 1178-3 on "Experimental Electron Density as the key to understand chemical interactions".
2008	Main Organizer along with Dr. Piero Macchi of the 5 <sup>th</sup> European Charge Density Meeting (ECDM-V) (6-11 June 2008), Gravedona, Como, Italy) (>180 participants)
2006-2007	<b>Chair</b> of the 2007 Gordon Research Conference (GRC) on Electron Distribution & Chemical Bonding. Co-chair was Dylan Jayatilaka, Australia
2003-2004	<b>Co-chair</b> of the 2004 GRC on Electron Distribution & Chemical Bonding. Chair was John Spence, USA.

1996-up to now	<b>Chair or co-chair</b> of 6 Microsymposia at IUCr Congresses, ECA (European Crystallographic Association) Congresses and Sagamore Conferences
1992-up to now	370 times Referee for 66 major international journals. <b>Awarded TOP 1% Peer Review for Chemistry</b> (2018 Peer Review Awards, Publons, <a href="https://publons.com/researcher/1336740/carlo/">https://publons.com/researcher/1336740/carlo/</a> )
2004-up to now	Referee for the Deutsche Forschungsgemeinschaft, the French National Agency (Agence Nationale de la Recherche, ANR), The French National agency for the scientific evaluation (ANRES, Agence National Recherche Evaluation Scientifique, the US National Science Foundation (NSF), the US Department of Energy (DOE); the Swiss National Science Foundation, NSERC Canada, University Western Australia, the Research Foundation-Flanders, F.R.S.-FNRS (Belgium), national Science Center Poland, etc
2000-up to now	External Referee of 23 international PhD theses and of 21 career promotions or prizes of foreign researchers; 12 times also member of Jury for foreign PhD theses
1981-up to now	Principal investigator of a number of European and National research projects, including two European Community projects

## Honours

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2013 Gregory Aminoff Prize and Medal (Royal Swedish Academy of Sciences, the Nobel prize Academy)	Carlo Gatti has been awarded the <b>Gregori Aminoff Prize 2013 from the Royal Swedish Academy of Sciences</b> , along with Prof. Mark Spackman. See for details: <a href="http://www.kva.se/en/Prizes/Gregori-Aminoff-Prize/">http://www.kva.se/en/Prizes/Gregori-Aminoff-Prize/</a> . This prestigious prize is intended to reward a documented, individual contribution in the field of crystallography, including areas concerned with the dynamics of the formation and dissolution of crystal structures. Some preference should be shown for work evincing elegance in the approach to the problem. The Gregori Aminoff Prize was awarded for the first time in 1979 to Paul Peter Ewald and includes among its recipients, two subsequent Nobel Prize winners. The last is Dan Shechtman, Gregori Aminoff Prize 2000 for the discovery of quasicrystals and recipient, for this same discovery, of the Nobel Prize for Chemistry in 2011.
2014 Istituto Lombardo Accademia di Scienze e Lettere	Appointed as "Socio corrispondente residente" Istituto Lombardo Accademia di Scienze e Lettere, since 2 October 2014

## Research

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h-index	46 (ISI-Web of Science); 52 (Google Scholar)
Citations	7139 (ISI-Web of Science); 9894 (Google Scholar), December 2021
CG is included in the 100.000 top scientists in the world	Classified at <b>33509<sup>th</sup> ranking</b> (database for 2017 only, <a href="http://dx.doi.org/10.17632/btchxktzyw.1#file-b9b8c85e-6914-4b1d-815e-55daefb64f5e">http://dx.doi.org/10.17632/btchxktzyw.1#file-b9b8c85e-6914-4b1d-815e-55daefb64f5e</a> ) and at <b>50208<sup>th</sup> ranking</b> (database from 1996 up to 2017, <a href="http://dx.doi.org/10.17632/btchxktzyw.1#file-ad4249ac-f76f-4653-9e42-2dfebe5d9b01">http://dx.doi.org/10.17632/btchxktzyw.1#file-ad4249ac-f76f-4653-9e42-2dfebe5d9b01</a> ) see: Ioannidis JPA, Baas J, Klavans R, Boyack KW (2019) "A standardized citation metrics author database annotated for scientific field", PLOS Biology 17(8): e3000384. <a href="https://doi.org/10.1371/journal.pbio.3000384">https://doi.org/10.1371/journal.pbio.3000384</a>
CG is included in the Top Italian Scientists in Chemistry	<a href="http://www.topitalianscientists.org/TIS_HTML/Top_Italian_Scientists_Chemistry.htm">http://www.topitalianscientists.org/TIS_HTML/Top_Italian_Scientists_Chemistry.htm</a>
Peer-reviewed publications on International journals	133 (including one Nature paper and an addendum to the paper, also published on Nature, two Nature Chemistry papers and one Adv. Material paper)



Papers in books	14 published book chapters on international peer reviewed books
Edited books	1 edited book along with Piero Macchi on "Modern Charge Density Analysis", Springer 2012
Software	Author (TOPOND-98) or co-author (TOPXD, XD, NCI-Milano) of four worldwide distributed SW packages for charge density research; author, along with Silvia Casassa of the electron density topological code inserted in CRYSTAL-14 and CRYSTAL-17 releases
Lectures	63 Invited lectures in international conferences and 9 in national conferences (29 plenary lectures, all except three delivered abroad), plus 20 invited seminars abroad and 16 lecture at international schools
Discussion leader at GRCs	4 times discussion leader at Gordon Research Conferences (GRCs)
Peer-reviewed Conference Proceedings et alias	11 publications in peer reviewed conference proceedings and 17 more publications (see list)
Industrial/technical reports	3 industrial reports; 2 technical reports

## Areas of expertise relative to the main themes of CNR-SCITEC

### CNR-SCITEC:



### MY OWN EXPERTISE:

**Green Chemistry:** New generation, green, heavy-atom-metal free, organic-based electrodes Li/Na batteries; Novel Thermoelectric materials

**Chemistry and Energy:** Novel Thermoelectric Materials and new generation of organic electrodes Li/Na batteries

**Advanced materials:** Novel Thermoelectric Materials and Phase Change Materials

**Theoretical/Computational Modeling:** it may naturally include all my work (modelling, computational and code development activity)

### Research objectives

During the years, my research has touched several fields, ranging from developments in theoretical and computational chemistry, to analyses of charge and spin densities in vacuo and in condensed phase (especially crystalline systems), to materials science.

In spite of the diversity of the topics I afforded throughout my career, a common trait has always characterized my efforts, namely that of carrying out theoretical "experiments" that could compare to or complement the outcomes from emerging new experimental techniques or new chemical applications, while focusing my main attention on getting a simple, yet rigorous, chemical insight from calculations, regardless of how complex they could be. A direct comparison of theory to experiment requires that one adopts a common tool of analysis of the obtained results, while removing all the unnecessary methodological differences that would customarily preclude a meaningful assessment. This prompted me to develop software tools for the analysis and/or the evaluation of experimentally detectable observables, like the electron density, or to propose new chemical descriptors, such as the Source Function, also based on a physical and measurable observable. A list of the main computer packages I've been developing is reported at page 11.

A general survey on part of my activity is given in paper n. 61, entitled "Chemical insight from electron density and wavefunctions: software developments and applications to crystals, molecular complexes and material science (Theor. Chem. Acc. 117, 847-884 (2007)) and also in the review paper (paper n. 85) I've been invited to write for an issue of *Physica Scripta* celebrating the Gregory Aminoff Prize 2013 (awarded to Mark Spackman and myself).

In the following, I will concisely summarize those aspects which **have or have had more relevance to crystallography, due to the fact I've been awarded a very important international prize in this research area. A more general overview of my research achievements may be deduced from the list of published papers. Numbering of cited bibliography, denoted as [xx] for papers and as [xb] for chapter books, refers to the full list of my peer-reviewed papers and book chapters.**

### **Early discoveries and developments of charge density topology:**

Back in 1984, I became interested in the work by Richard Bader on the topology of the electron density in vacuo and on the related Quantum Theory of Atoms in Molecules (QTAIM) he was developing in that period. My first work in the area [6,8] had already a "*crystallographic*" imprint since I could show that the different geometrical structures found in a number of crystals of 11,11- Disubstituted 1,6-Methane [10] annulenes could be assigned to either a dinorcaradienic or a [10]-annulene type depending on the features of their electron density topology. Moreover, I showed that differences in the matrix effect could be strong enough to stabilize in two different structural forms, one having dinorcaradienic, the other annulenic character, the two albeit chemically equivalent molecules in the crystal unit cell of the dimethyl derivative [6].

Later on, I made the unexpected and important discovery [11,12] that non-nuclear attractors may occur in the charge distribution of some peculiar systems. This observation had a great impact, since it was in seemingly contrast with a basic assumption of QTAIM, according to which the nuclei are the only maxima in the molecular and crystalline charge distributions and thus may act as the sole 3-dimensional attractors of the gradient of the electron density field. Although in most molecules nuclei are indeed the sole attractors of the charge density and the atomic form is dominant, I have shown that there are systems, both in vacuo and in condensed phase where maxima at position other than nuclei also occur. These maxima were called nonnuclear attractors (NNAs) [11] and the union of a NNA and of the  $R^3$  space traversed by the gradient paths terminating at the attractor, was termed a pseudoatom because its behaviour mimics that of a regular atom in a molecule, but it cannot exist in isolation [11,12]. I showed that QTAIM had not to be modified, but simply generalized to systems where besides the usual atomic basins enclosing a nucleus, pseudo-atoms also occur [11]. Despite being now well-established and accepted in literature, NNAs still raise significant interest and are increasingly being found, in particular in systems under high pressure, like in a recently discovered insulating structural phase of Na (*Nature* **458**, 182-185). The first example reported in literature where the occurrence of NNAs was not due to inadequacies of the adopted computational level was the  $\text{Li}_2$  molecule and the Li planar clusters [11]. In these systems, bonding through lines of maximum density with respect to lateral displacements (the so called bond paths) never occur between the Li nuclei, but only between Li nuclei and NNAs or between the NNAs themselves, which so provide the "glue" ensuring stability to such systems. Later on, with Bernard Silvi, I also showed [35] that a close correspondence between the occurrence of NNAs in metal and clusters, and the localization of electrons in interstitial regions of these systems, as determined by the Becke's Electron Localization Function (ELF) topology, exists. An unexpected but distinct feature of the electron density distribution, namely the occurrence of NNAs, was so nicely put in relation with a property determined through a more complex, two-electron function, the pair function, a function strictly related to the instantaneous, rather than to the average, correlated motion of electrons. Along with Georg Madsen et al [33], I also demonstrated that the F-centers occurring in some crystalline systems may be put in 1 to1 correspondence with NNAs, representing indeed one of their possible physical manifestation.

A throughout study [13] of the effect of the electron correlation on the charge density topology of molecules was another important development I made to QTAIM. Thus far QTAIM had been applied only to Hartree-Fock wavefunctions, including Fermi correlation only. During my visits to Richard Bader's lab In 1986-1987, I decided to extend the topological programs to the Coulomb-correlated wavefunctions, such as

those obtained with the CI, MCSCF and GVB methods, so as to allow the effect of the static and dynamic Coulomb correlation to be also evaluated. In the same years, I also contributed to an important paper on molecular dipole moment decomposition and molecular dipole moment changes under vibration [10]. This work also provided a clear and quantitative insight on the approximation inherent to the rigid pseudoatom approximation customarily adopted in experimental charge density study, where the pseudoatoms density is assumed to rigidly follow the motion of the nucleus it is attached to.

### **Bridging the gap between the analysis of experimentally and theoretically derived electron densities:**

The origin of this part of my work dates back to 1990, when Riccardo Destro and coworkers had obtained in Milano an experimental electron density distribution (EDD) of excellent quality for the zwitterionic amino acid L-alanine, starting from an extensive set of single-crystal X-ray diffracted intensities measured at 23 K (J. Phys. Chem. **92**, 966-973). The very low collection temperature made the thermal diffuse scattering negligible and minimized the problems associated with the deconvolution of the static charge density from the mean thermal vibrational distribution of the nuclei, enabling the measurements of extensive sets of data, far beyond the limits usually encountered at room temperature. The L-alanine X-ray data set was thus an ideal candidate for deriving not only the standard difference-density maps of crystallographers, but also the *total* charge density distribution [19,20]. Experiment and theory were then becoming directly comparable, provided one had adopted an interpretive tool based on the observable that experiment and theory were both determining, and regardless of the different tools - pseudoatom multipolar models or Molecular Orbitals like models – used to extract such a observable. Electron density topology and the underlying QTAIM was the proper method to be used. It would have not only provided a common framework of analysis, but also one able to give precious chemical insight. In 1992, I published a paper on the experimental vs theoretical topological properties of charge density distributions in the L-alanine molecule [20]. Gladly, experimental and theoretical distributions showed the same number and type of critical points (CPs) in the electron density. However, as far as the CP locations and the CP properties (electron density, its Laplacian and curvatures) were concerned, a very close agreement between theory and experiment was found only for the non polar C-C bonds, whereas for more polar interactions like C-O and C-N bonds noteworthy discrepancies were observed. The paper focused on the factors influencing the theoretical topologies, such as the basis set quality, the inclusion of electron correlation and of the crystal-field effects (limited to a molecular cluster approach) and compared the corresponding results to those derived from a number of optimum least-squares refined experimental densities or to those obtained from the very crude independent-atom model. This work aroused some interest and Prof. Philip Coppens, in his review paper entitled the *Charge Density Analysis at the Turn of the Century* (Acta Cryst A **54** 779-788), reckoned my paper as a “pioneering, first systematic topological analysis using both experimental and theoretical results”. I felt however uneasy with the too crude treatment of the crystal field effects adopted in my theoretical calculations. Indeed, and quite unexpectedly for me at that time, the intramolecular bond critical point (BCP) properties seemed not to have reached convergence despite the use of an apparently reasonable number of molecules in the cluster approach, whereas, the intermolecular BCP properties had converged even at the very crude molecular dimer model level. Therefore, I thought it mandatory to develop a tool which could enable one to apply QTAIM directly to the periodic wavefunctions of the crystals. Roberto Dovesi, Cesare Pisani and Carla Roetti at Turin university, along with Vic Saunders and Nick Harrison at Daresbury (UK) were then developing the upcoming 1995 version of their CRYSTAL package, which would have included for the first time both RHF and DFT, along with direct SCF capabilities, in a fully periodic code. These were decisive improvements in view of a comparison with the fast increasing quality of the experimental EDDs. The groups in Turin and Daresbury asked me to join them in a European project aimed at the “*Development and Applications of the Hartree-Fock Method to Materials Science*”. Within this program, I wrote the code TOPOND-96 [25], the first distributed QTAIM implementation for periodic systems in 0 up to 3 dimensions, so covering in just one code the case of molecules, polymers, surfaces and crystals. The following release of the package, TOPOND-98 and its recent updates are described in [61,6b], whereas Ref. [38] illustrates the features of TOPXD – the TOPOND interface to the XD multipolar package enabling one to exploit the specific TOPOND capabilities for experimental densities also, which I developed along with Anatoly Volkov and Philip Coppens in Buffalo. Now TOPXD is fully inserted in the XD-2006 package, the most popular and probably the most efficient package for Multipole Refinement, Topological Analysis of Charge Densities and Evaluation of Intermolecular Energies from Experimental and Theoretical Structure Factors. This code, of which I'm a coauthor for the part related to TOPXD, has been distributed in over 100 international labs.

Applications of TOPOND to the realm of molecular organic crystals paved the way to the interpretation and quantitative evaluation of the effect of packing on molecular EDDs topologies [25,26,43-44], and on other molecular properties, like in particular the molecular dipole moment [25-26,43] or the electric field gradient (EFG) at nuclei [24]. By applying QTAIM on crystalline and in vacuo EDDs and using the same computational (CRYSTAL-XX) and topological codes (TOPOND), I could demonstrate and quantify



the impressive enhancement of molecular dipole moment occurring in many hydrogen-bonded systems, caused by the matrix effects. Dipole moment enhancements in Ice VIII [26] and urea [25], with respect to the corresponding molecular systems in vacuo, amounted to about 25 and 37%, respectively. I could also characterize [43-44] the peculiar *nature* and *function* of the CH...O intermolecular interactions in a crystal presenting only this kind of intermolecular bonds, whose appreciation as weak, but not negligible, hydrogen bonds had for a long time been debated and even denied in the literature. I was able to show that the weak CH...O interactions may have a very important role as, for instance, in some crystals, they are able to induce a molecular dipole moment enhancement [43] that is comparable to and in most cases even much larger than that found in systems packed together by the stronger OH...O and NH...O bonds. Furthermore, I could provide a simple qualitative and quantitative explanation for such an unexpected behavior.

The earlier mentioned discrepancies between experimental and theoretical EDDs topologies did not in general vanish with inclusion of a proper evaluation of the crystal field. The major reason had to reside somewhere else. Through a fruitful cooperation with Philip Coppens and Anatoliy Volkov at SUNY-Buffalo (US), and using CRYSTAL, TOPOND and TOPXD codes in combination, we could demonstrate [38-39] that it is mostly the limited flexibility of the radial functions used in the multipolar analysis that often bias significantly the topological experimental results. Indeed, the observed discrepancies were generally found to significantly decrease when the theoretical densities were projected into the multipole densities functions through refinement of the theoretical structure factors.

### Chemical bonds in crystals

As already in part outlined, a common trait of my research has always been the study of chemical bonding, with a particular interest in understanding how atoms get bonded to one another in non conventional situations and in how the environment influences, in general, such bonding. I already mentioned the specific software developed to extend QTAIM to correlated wavefunctions and to the wavefunctions of periodic systems. Examples of systems with peculiar bonding properties are those characterized by the presence of NNAs, bond or point defects, F-centers [11-12,29,36,33]. Or bonding in metals [35], surfaces [34,42,61], inclusion compounds like the inorganic clathrates [48] having promising thermoelectric properties or the organometallic complexes [27,58,69], showing relevant catalytic features [64]. Not less important intermolecular bonding, like the CH...O bonds [43-44], or the effect of environment in biologically relevant systems [74].

In 2004 Artem Oganov, as guest editor of a Zeitschrift fuer Kristallographie issue dedicated to Computational Crystallography invited me to write a review on the study of chemical bonding in solids. This 59 pages review, significantly entitled *Chemical Bonding in Crystals: new directions* [57] has been well-received (over 450 citations thus far) and, besides providing a detailed and wide panorama of the development of the field, also testifies my own contribution to it along with that of others. Later on, in 2007, I was asked by Artem Oganov to help him in characterizing and studying the peculiar bonding features and internal charge transfer of a new phase of boron at high pressure, found through his evolutionary crystal structure prediction method. At low pressures (<19 GPa) boron adopts covalent structures based on icosahedral B<sub>12</sub> clusters, while at high pressures (>89 GPa) had been predicted to form a superconducting  $\alpha$ -Ga-type phase. Besides proving this latter high-pressure phase, we characterize, between 19-89 GPa, an hitherto stable, unknown structure,  $\gamma$ -B<sub>28</sub>, consisting of icosahedral B<sub>12</sub> clusters and B<sub>2</sub> pairs in a NaCl-type arrangement [65]. A surprising finding was that the bonding between the B<sub>12</sub> clusters and the B<sub>2</sub> pairs is partially ionic [65,68], as suggested by the infrared spectrum of the polymorph and supported by the theoretical calculations and in particular by the charge density analysis I performed, which could also explain the origin and direction of the observed charge transfer [65]. This was the first documented case of a partially ionic crystal made of just one chemical element, with the B<sub>2</sub> and the B<sub>12</sub> clusters playing similar roles to "cations" and "anions" in normal ionic salts. The new phase turned out to be a key to understand the phase diagram of boron – the only element for which the phase diagram was unknown since its discovery 200 years ago. This exciting study, published on *Nature* [65] has been favorably received, >700 citations and commented (see for instance, John Tse, *Nature*, News and Views, 457, 800-801 (2009)).

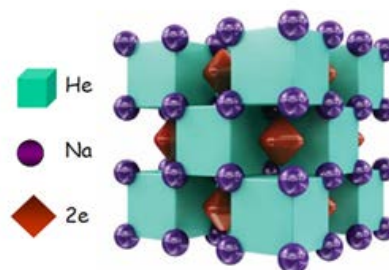
Another quite interesting and more recent case concerns the discovery of the first neutral thermodynamically stable (at P >113 GPa) compound of He, Na<sub>2</sub>He, published on *Nature Chemistry* [104]. It has been discovered using a variable-composition evolutionary crystal structural prediction approach (implemented in the Uspex code by Oganov), followed by experimental validation and rationalization of its geometrical & electronic structure in terms of quantum chemical topological methods. Na<sub>2</sub>He resembles a 3D checkerboard with Na<sub>8</sub> cubes alternatively filled with He or allocating an interstitially localized electron pair, revealed by a non-nuclear attractor electron density (ED) maximum and a massive accumulation in the deformation ED map. Na<sub>2</sub>He is an electride, with localized electron pairs forming 8c-2e bonds within the empty Na<sub>8</sub> cubes. This work has been commented in several sources including C&En newsletter (volume 95, Issue 7, p. 5, 2017) where one may interestingly read the following: "Chemistry textbook authors may soon have to rewrite

sections covering noble gases and chemical inertness. An international research team has reported the synthesis of a helium-sodium compound that's stable at high pressures.... ; besides, Lund University inorganic chemist [Sven Lidin](#), has remarked that "regarding our perception of chemical reactivity, this is a textbook changer." Earlier discoveries of other noble gas compounds made it clear that inertness is a question of reaction conditions.... But helium has been a holdout even under extreme conditions because it clings to its inner-shell electrons tightly and will not let go. These new findings show that in some ways, "**the last bastion of inertness has finally fallen**." The work on Na<sub>2</sub>He has been well received and it has already been cited over 130 times since its publication in 2017.

## Na<sub>2</sub>He

Nature Chemistry **9**, 440-445 (2017)

Paper n. 104



You may also enjoy reading my divulgative paper [publication n. 8, section "other publications"] on the fascinating aspects of the new chemistry that reveals itself under high pressure, which I wrote in 2019 for the Istituto Lombardo Accademia di Scienze e Lettere after giving a conference on "Tavola periodica sotto pressione: una periodicità diversa ed una chimica esotica" on occasion of the 150 years from the discovery of Mendeleev's Periodic Table of Elements.

### New bonding descriptors. The Source Function: a tool to extract chemical information from theoretical and experimental electron densities

One of my privileged lines of research in the past ten years has been the development of the Source Function descriptor that Richard Bader and I introduced back in 1998 [31]. The Source Function (SF) enables one to view chemical bonding and other chemical paradigms from a totally new perspective and using only information from the electron density observable and its derivatives. This function equates the value of the density at any point within a system to a sum of atomic contributions and it is completely independent from the tools used to obtain the electron density, which may be either derived through experimental techniques such as X-ray diffraction or with one of the many available quantum mechanical models at different levels of complexity. I've published on Structure and Bonding [75] a very comprehensive and long (93 pages) review on the SF, along with a description on all the ongoing developments on this function I'm presently working on. Although not deliberately put forward for such a purpose, the SF permits to get through one of the most debated aspect of QTAIM one which is customarily considered as an intrinsic limit of the theory. Within QTAIM, a bonding interaction between two atoms is associated to the presence of a line of maximum density, that is a bond path (BP), linking their nuclei at electrostatic equilibrium. However, a BP is topologically associated to the only two atoms it connects and it is thus inherently unable to directly visualize an interaction involving more than two centres, despite both the BP occurrence and its shape depend in principle on the whole set of physical interactions present within a system. The SF unveils such dependence, by pointing out which other atoms, besides the two connected by the BP, significantly contribute to the observed density accumulation along the path and, in particular, at the BCP. Other bonding descriptors, like the QTAIM delocalisation index or the synaptic order of an ELF valence basin give access to *non-local* information on bonding and on complex, unconventional bonding patterns. A distinctive feature of the SF with respect to these two powerful interpretive tools is that it is directly amenable to experimental determination, as due to its intimate link with the system's electron density Laplacian. This puts the SF in a privileged position for retrieving comparative bond information from experimental and theoretical results. The SF has been shown to be able to mirror the chemical bonding nature [75, 46,54,58,61,6b] and [73] to be able to neatly reveal electron conjugation effects, including  $\pi$ -electron conjugation, directly from the electron distribution and independently from any molecular orbital scheme or decomposition. This hold true also for X-ray diffraction experimentally derived electron densities [98]. Source Function applied to experimental densities was demonstrated to reveal subtle electron delocalization effects and to be able to appraise their transferability properties in crystals [98]. The SF is becoming progressively well-known [75] and it has been implemented in the latest version of the XD package, as well as in a code for the topological analysis of

theoretical wavefunctions and densities. Through the years the SF has been exploited by me and by a growing number of crystallographers to assess chemical transferability [46, 98] or to describe chemical bonding in challenging situations, like for instance the short-strong hydrogen bonds in  $\pi$ -conjugated frameworks [46,75] or the metal-metal and metal-ligand interactions in the crystals made of organometallic complexes [58,64]. The local SF, if integrated also over the position of the reference electron, enables one to define a full population analysis [75]. This would allow to completely overcoming any arbitrariness related to the various population analysis scheme existing to date. I published preliminary results using such a fully unambiguous population analysis [75]. However very unpleasant numerical problems need to be solved before the method may be considered applicable in every circumstance. I could also show [67] how robust is the SF descriptor against changes in the models used to derive electron densities from theory of experiment. I'm currently working on more widely exploring the capabilities of the SF to reveal electron conjugation effects and on the possible ways of further decomposing the atomic SF in chemically meaningful additive pieces, like core and valence atomic contributions, without introducing any specific model, but simply exploiting information from the electron density or its Laplacian observable [75].

Very recent applications of the SF tool concern two studies aimed at probing cyclic  $\pi$ -electron delocalization in N-heterocyclic carbenes [110] or at revealing the locality extent of the hydrogen bonds of the DNA base pairs in their neutral and ionized ground states [109].

Of particular interest are the recent developments concerning the extension of the SF to the electron spin density [96,11b] and to the electrostatic potential (EP) [108,118]. The first extension enables one to have precious insights on the way spin density information is transmitted in a molecular system [106,107]. Hence it is of particular relevance for the study of magnetic systems and magnetic phenomena. The second extension, instead, enables to detail the weight that various portions of a system have in producing the value of EP in its positive maxima associated to the sigma or pi-holes associated to chalcogen, pnictogen and halogen bonds. These holes are of great relevance in the molecular recognition processes driven by intermolecular interactions based on such linkages. The SF extended to the EP finds a promising application in the field of the enantiomeric separation through HPLC (High-Performance Liquid Chromatography) techniques [108,118].

### **Source Function for the electron spin density**

Modelling magnetic properties of crystalline compounds by experiments is truly challenging. New methodological routes are now available to ease this task. By combining the information obtained by different techniques such as X-ray and polarized neutron diffraction (PND), or PND and X-ray magnetic diffraction, the limitation of the scarce number and resolution of experimental data is partly overcome. More precise wavefunction-based models or electron spin densities (SDs) are so obtained and comparison with *exact* wavefunctions or densities becomes clearly advisable to test their accuracy. *Ab-initio* electron SDs can be easily calculated but they are usually far from being reliable. Systematic studies demonstrated that DFT is often unable to treat open-shell systems properly, leading to non-accurate electron SDs. *Ab-initio* electron correlation methods or density-matrix renormalization group approaches, have to be called for. Yet, they are often computationally too demanding and unsuited for large systems. On top of all this, *extraction of chemical information from the SD is not a trivial task* as it is for the electron density (ED), even for very simple molecular systems. Yet, understanding how spin information is transmitted from paramagnetic to non-magnetic centers in a molecular or condensed phase system is crucial in advanced materials research and calls for novel interpretive tools. To follow this aim, I have extended the Source Function tool to the case of the electron spin density [Chemical Science paper, 96 and 11b]. I could so show that the spin density at a point may be seen as determined by a local source operating at all other points of space and that integration of the local source over atomic basins allows for measuring their contribution in setting the spin polarization at any system's location. I also showed how to conveniently decompose each atomic contribution in a *magnetic* term due to the magnetic natural orbital(s) density and in a *reaction* or *relaxation* term due to other orbital(s) density, both terms largely concurring to enhance the chemical insight on magnetic behaviour provided by this newly developed interpretive tool. I purposely wrote a new set of codes for implementing this interesting extension of the SF tool, introducing also the new **concept of partially SF reconstructed electron or electron spin densities**. [106] At variance with the standard SF percentage representations, such reconstructions offer a simultaneous view of the sources originating from specific subsets of contributing atoms, in a selected molecular plane or in the whole space and are therefore particularly informative.

The newly developed SF tool has been used to analyze the magnetic patterns in organic systems [11b] and in metal complexes molecular crystals, in particular two azido di-copper complexes, one weakly and one strongly ferromagnetically coupled [106,107]. The SF SD serves as a useful tool for discussing the SD

accuracy and for disclosing the origin of the SD discrepancies when approaches of increasing quality are used. The SF has enabled to highlight the origin of the SD differences between the two di-copper complexes and among the adopted computational approaches (CASSCF, UDFT, UHF). DFT methods were found to exaggerate electron sharing between Cu and the ligands, leading to spin delocalization towards them and to an overestimation of the metal-ligand spin polarization. At the same time, DFT underestimates the spin information transmission between atoms, relative to the CASSCF method. PND SD is closer to CASSCF SD than to DFT SD. I also analysed whether it is DFT overdelocalizing spins, or is it a consequence of DFT overdelocalizing the charge, exploring ways, if any, to untangle the two effects [107].

### **Source Function for the molecular electrostatic potential**

Enantioseparation on chiral stationary phase (CSP) is based on the formation of transient diastereomeric selectand-selector complexes in a chiral environment generated by a chiral selector. Diverse short-range directional interactions, including hydrogen bonds,  $\pi$ - $\pi$ , dipole-dipole, and van der Waals interactions, underlie complex formation and promote the enantioseparation. In this context, recently, it has been discovered that  $\sigma$ -hole interactions can be involved in HPLC enantioseparations, enlarging the range of interactions with are active in this environment. Computational tools and studies *in silico* have greatly contributed to the understanding of  $\sigma$ -hole interactions. In particular,  $\sigma$ -hole being a region of electronic charge depletion, electrostatic potentials (EPs) have been widely used as an indicator of the anisotropy of the molecular charge distribution. While it is well acknowledged that  $\sigma$ -holes originate from the cylindrical symmetry of the  $\sigma$ -bond and of the electron sharing along its axis, none is quantitatively known about the role played by the various moieties of a molecule in producing such holes. I have thus extended the SF tool to the EP, to yield a rigorous measure of how the various pieces of a molecule determine the extent of  $\sigma$ -holes as measured by the EP value at their associated EP maxima on the 0.002 au ED isosurface. A package of several intertwined FORTRAN codes was developed for such a purpose. A first application of the EP SF tool to the chalcogen bonds in HPLC enantioseparations of fluorinated bipyridines has been published [108], along with a general survey on the use and on deciphering the role of halogen bonds in separation science [118].

### **Bond path and beyond:**

During the last 10 years, it has become evident that the bonding classification schemes derived from the various topological approaches need to be critically analysed and even revised if metal-metal (M-M) bonds or metal-ligand (M-L) interactions are addressed [57,58,69,75]. Since the electron density topological approaches play a central role in the study of bonding using EDDs derived from X-ray diffraction [57], this has also become a challenging and timely issue for the study of bonding in crystals. Problems involve in a first instance the choice of a suitable criterion to establish which atoms are actually bonded to one another – eventually leading to the so-called “molecular structure” – and, secondly, the characterization and classification of the resulting chemical bonds. When translated to common “chemical thinking”, the very successful and “universal” bond path (BP) criterion which defines whether or not two atoms are bonded to one another appears, in the case of organometallics, not completely free of limitations. For these systems, continuous rather than discontinuous bonding indicators and descriptions seem to be perhaps more appropriate [57,75]. Very soft potential energy surfaces – hence often very flat electron densities – characterize the M-M and M-L interactions, so that the resulting structural diagrams exhibit an enormous sensitivity to computational or experimental details. And, as a consequence, the presence or lack of these interactions, when judged solely by the bond path criterion, may in some instance be a rather subtle and controversial issue. This observation is obviously tied to the intrinsic inability of the bond path criterion to directly detect multicenter bonding (see discussion on the SF). By using the BP criterion, bonding through the bridging ligands and direct M-M bonds are usually alternative and competitive options, but they are not necessarily so when continuous descriptors of bonding are adopted.

I've afforded this debatable matter by trying, on the one hand, to understand what the occurrence of a BP exactly means from a physical point of view and by developing, on the other hand, several investigative tools, able to provide an alternative or complementary view of bonding with respect to the usual BP criterion. Along with Angel Martín Pendás, Miguel Blanco and Evelio Francisco in Oviedo and using their Interacting Quantum Atoms (IQA) theory, we have demonstrated [62] that bond paths must be interpreted as privileged exchange channels – an important conceptual progress which easily explains why under certain chemical circumstances a bond path may either be present or not despite the existence of a significant electron sharing between two interacting atoms. This interpretation was strongly supported by the interesting observation that when two pairs of atoms are competing for a bond path, the pair found to be linked by a

bond path is always the one with prevailing contribution of exchange energy. Indeed, we showed that for systems evolving through conflict mechanisms, the exchange energy curves of two competing pairs cross almost exactly at the conflict catastrophe point, where a switch from a bond path linking one pair to one linking the other pair precisely occurs. I believe that much of the current arguing on BPs and on their relationship to “chemical bonding” might be probably calmed down if such an extended vision of the BP meaning would be taken in some consideration, if not fully embraced.

Along with Robert Ponec I've also shown [69] how the domain averaged Fermi Hole (DAFH) analysis could be another very useful interpretive tool in the area. For this purpose we generalized and extended DAFH theory to the QTAIM atomic domains, with boundaries defined in real space and through the electron density observable [69,72]. When applied to the highly debated case of the triply-bridged  $\text{Fe}_2(\text{CO})_9$  coordination complex, where the 18-electron rule would predict a direct Fe-Fe bond, the DAFH approach rather than this direct M-M interaction suggests the existence of a multicenter 3c-2e character of the bonding of the bridging ligands [69]. This view nicely fits with the non negligible electron sharing found between the two metal atoms, despite the absence of a direct Fe-Fe bond, since the existence of non-vanishing delocalization indices between all pair of atoms has been proved to be a necessary requirement for the presence of 3c-2e bonding in any A-B-C fragment.

Another tool, able to overcome the problems inherent to the possibly discontinuous description of bonding provided by the electron density topology and the bond path criterion, is clearly the SF, I mentioned earlier and which is now being extensively used in literature to discuss bonding. SF applications to the organometallic systems, including mine [58,64,75], were well received in literature. Although lacking the very important physical meanings associated to either the delocalization indices or the IQA, DAFH and ELF analyses, the SF has the great advantage of not requiring the pair density (or at least the first density matrix if single determinant theoretical approaches are used) for its application and for being so, as mentioned earlier, immediately applicable to both experimental and theoretical electron densities. This is an important mark since until recently the most decisive features of the experimental studies of bonding in organometallics were often derived from complementary theoretical calculations – a situation which clearly raises the question of whether or not it is indeed worth performing the more time consuming experimental determinations for such systems.

### **Clean and covered surfaces: reconstruction and bonding**

Owing to its intimate link with the CRYSTAL package, TOPOND can be naturally used to study 2D periodic systems, like a slab cut from a bulk system along a given crystalline face and then either preserved as a clean surface or allowed to be chemisorbed by suitable chemical passivating species. In a 1996 Chemical Review paper on the semiconductor surface reconstruction [Chem Rev **96**, 1237-1259], Charles Duke developed the point of view that the “surface regions of tetrahedrally coordinate semiconductors form new 2D compounds whose bonding, constrained by the requirement of epitaxy with the substrate, exhibits properties distinct from either the corresponding bulk solids or molecules based on the same atomic species”. I clearly thought that TOPOND was the right tool to discuss bonding in these “new 2D compounds” and in a way set to be suitably compared with experiment, once the first accurate and extensive data sets would have eventually become available. Issues like the following could with TOPOND be quantitatively addressed : how is the bonding of surface atoms affected? What is a “dangling” bond and how is modified by surface reconstruction? Why does a surface reconstruct? How rapidly do the surface perturbations and the changes in these perturbations that result from the reconstruction or adsorption process decay into the crystal in terms of the properties of the atoms in each of the succeeding layers? What are the charges on the surface atoms in a free surface and in the chemisorbed states? How much electronic charge is transferred and in what direction? What is the atomic origin and nature of the surface “double layer”? Along with Fausto Cargnoni, I could provide interesting answers to all these questions, by applying the method to the Si(111)(1x1) clean and H-covered surfaces [34], to the Si(111)(2x1) reconstructed surface [42] and to the Si(100) clean and H-covered surfaces [61].

### **Materials Science and Crystallography**

I have also taken part to cooperative projects in materials science, addressing problems intimately related to some specific structural and electronic features of materials in crystal phase. Atomistic modelling lies at the bottom length-scale of the multiscale modelling computational approach to materials science. Knowledge of how atoms bond to other atoms, how impurities, doping or atomic substitution affect this bonding, and how bonding, cohesion energy, and the ensuing bulk material properties relate among each other is a typical outcome of an atomistic-level simulation. However, bonding in pure or defective solids or in complex supramolecular aggregates can not often be easily interpreted with standard methods of bond analysis and the use of QTAIM, a method firmly rooted in physics, and not based on any preconception of bonding, has proved to be particularly helpful in this case.

Along with Luciano Colombo (INFM, Milano) I addressed the structural and bonding problems related to the migration and interaction of native point defects in silicon, a phenomenon affecting many, industrially relevant, micro- and mesoscopic properties of silicon bulk samples. Our studies on a kind of bond defects, arising from the incomplete recombination of vacancy-interstitial pairs in silicon [29], and on our interpretation [36] of the structural and energetics evolution which takes place during the growth of self-interstitial clusters in the silicon crystal were very well received.

In the first decade of the 21st century, within the European Community project “*Nanothermel – High performance thermoelectric materials for heat recovery and cooling applications*”, I’ve been working on the relationships between the geometrical and electronic structure of thermoelectric materials (TEs) and their ensuing electronic transport properties [5b]. These may be obtained from the knowledge of the full band structure, using the semi-classical Boltzmann’s transport theory and the approximation of a constant relaxation time. Along with Luca Bertini, I developed a code, named ELTRAP (Electron Transport Properties), interfaced to the CRYSTAL-98 package. Given a newly synthesised TE material of known starting stoichiometry, it is very difficult, if not often impossible, to know its precise geometrical structure, not to speak of its exact composition. Furthermore, its TE properties are typically the result of the combined effect of the different geometrical structures and/or chemical local compositions characterizing the material. I showed that ab-initio theoretical modelling may produce several useful feedbacks. For instance, I have been able to show that the Seebeck coefficient and its trend with the temperature or with the doping level is a very precious structural informer [55]. More in general, theoretical modelling singles out the effects that a well-defined composition and general structure has on the geometrical, electronic and TE properties and it so allows for a rational design of improved performance materials [47,48,50,52,55,56,61,63,6b]. Theoretical modelling also provides a synergic help and a mutual validation between computed and multi-techniques experimental structural hypotheses, as testified by the fruitful cooperation [48,50,52,56] I had with the structural group at Aarhus University (DK), headed by Bo Iversen. Finally, I showed how ab-initio modelling can be used as guidance for design of optimum TE materials through the prediction of the best doping level based on the computed electronic transport properties [50, 6b]. A number of published case studies concerned novel promising TE materials such as the type I inorganic clathrates  $A_8Ga_{16}Ge_{30}$  ( $A=Sr,Ba$ ) [48], the Zn-Sb alloys [50] and the modified  $Co_4Sb_{12}$  skutterudite phases [47,52,53,55-56,61,63,6b]. In particular, in 2003, and contrary to the then available experimental evidences, I could demonstrate [48] the Zintl nature of the inorganic clathrates structures hosting alkaline-earth metal guests in their oversized cages. In 2004, along with the group of Bo Iversen in Aarhus we found the presence of Zn interstitial atoms in the “ideal” structure of Zinc antimonide and showed how they play a fundamental role as electron suppliers and Seebeck coefficient enhancers, as well as lattice thermal conductivity suppressors [50]. We could also suggest how the already excellent thermoelectric properties of Zn antimonide could be hopefully even slightly improved through a very small amount of electron donors dopants [50].

### **Phase Change materials. Relationship between their peculiar physical properties and unusual chemical bonding features.**

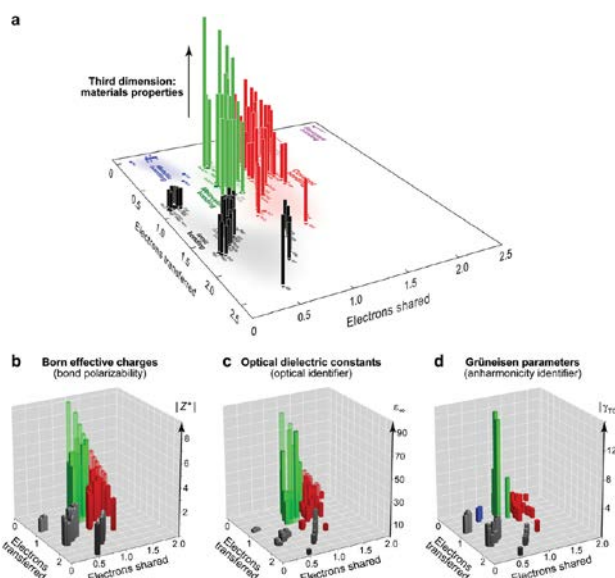
Chalcogenide phase-change materials (PCM) are widely used for data storage and photonics, as they can be easily transformed between their amorphous and crystalline states, having significantly different optical properties and a pronounced resistivity difference. This contrast of properties has been summarized in five specific fingerprints for PCMs crystalline states and reasoned in terms of *metavalent* bonding (MVB), a distinct mode of bonding which seems to characterize the crystalline phase. Since the changes observed upon crystallization concern either purely structural evidences or a set of dynamical and out-of-equilibrium properties, the important question arises of whether the PCM crystalline states entail specific features also in terms of bond characterizations based on electron distributions and bonding descriptors derived thereof [109]. A 2D map of bonding in solids was thus established by using electron sharing indices and charge transfer descriptors [109]. Peculiar combinations of their values lead to steep variations in a third dimension relevant to response material’s properties [109]. Though the necessity of calling for a new type of bonding in PCMs may be questioned, the small or large susceptibility to steep property changes emerges as a relevant feature of bonding, yet too often overlooked in usual bond descriptions.



## 2D (bonding) and 3D (Bonding+Properties) Maps for Designing promising Phase Change Materials

Adv. Materials Adv. Mater. **31**, 1806280 (6 pages) (2019)

Paper [109]



## Reshaping the old Linus Pauling's Bond Valence model for making it suited also to systems including metal-metal bonds [112,114,116,119]

Bond Valence Model (BVM) was introduced long time ago by Linus Pauling and it is still widely applied ( for instance, the book by I. D. Brown (2006) " The Chemical Bond in Inorganic Chemistry: The Bond Valence Model" has >1250 citations). The Bond Valence Model (BVM) is used in crystal chemistry to check the reliability of structure solutions and to determine cation oxidation states, for modeling of ionic transport in solids, in particular, in cathode materials for Li batteries, for accurate molecular dynamics simulations, etc. The unique BVM ability to calculate the bond strains from the experimental interatomic distances and relate them to material stability has been used for crystal structure predictions, in particular, for perovskites. BVM model has been also recently used to quantify the bond strains in cathodes for Li and Na batteries, showing that this method can predict and explain the material stability even better than traditional calculations of formation energy. It may be used also to describe the lattice strains in Chevrel Phases, well-known superconductors, ionic conductors and unique cathodes for Mg batteries.

**However, for a long time, the BVM was thought to be irrelevant for compounds with metal-metal bonds.** For example, F. A. Cotton wrote in a book: "It is a general qualitative rule in chemistry that bond lengths and bond orders are inversely related... However, there is no a-priori reason to expect that similar procedures will (or will not!) work in the very different realm of metal-to-metal bonds. Experience is the only test, and experience thus far has shown that M–M bonds cannot usefully be treated in such a way...We condemn as foolish and hopeless any effort to associate a unique, quantitative bond order with each and every metal-metal inter-nuclear distance."

Working with Elena Levi and Doron Auerbach (Bar-Illan University, Israel) we could recently show, instead, that the Cotton's statement is caused by annoying confusion between formal and effective bond orders (BOs) values, which may reach 1 valence unit in compounds with metal-metal bonds (due to a high steric effect). As a result, the general rule mentioned by Cotton is valid only for the effective BOs that can be found by DFT or BVM calculations, but not for the formal BOs used by Cotton. In a variety of studies, [112,114,116,119], having several purposes, we could demonstrate that the BVM model may be safely extended to systems including metal-metal bonds, provided one adopt reliable effective bond orders (taken by a systematic analysis and proper interpolation of ab-initio derived bond order data). We could so confirm the validity of two basic principles proposed by Pauling, namely, i) the exponential correlation between bond lengths of the metal-metal bonds and their *effective* BOs, and ii) BO conservation principle for the M(etal) atoms; thus confirming the applicability of the BVM for cluster compounds. Our papers are especially important for cluster chemists, because the traditional ignoring of the BVM deprives them of a very simple and useful method, which may provide unique information, unreachable by other methods.

## Organic-based electrodes for Li-ion batteries: computing-driven search of optimal metal-free electrodes (brief overview)

- Energy storage set-ups based on redox active organic compounds are realistic candidates as an alternative to the costly and environmentally unfriendly batteries relying on TM-based electrodes

- Some families of potential materials in such devices have already been identified including in particular carbonyl and carboxylate based compounds, oxo-carbon derivatives, or also free radicals, organosulfurs ...
- Efforts to improve their capabilities are desirable. Especially, increased cell voltage while preserving or enhancing energy density of the material is required. This implies devising compounds with molecular weight as low as possible combined with respectively lower and higher redox potentials for anode and cathode applications, compared to current ones
- Screening new molecules through computational modelling prevent very expensive and time consuming trial and error experimental tests.
- Theoretical studies have a twofold role: they help to design new systems with improved features but also enable to rationalize their properties

We use an integrated approach consisting of :

- DFT computations combined with a continuum SMD solvent model to evaluate the redox properties of a series of organic derivatives
- QTAIM (Quantum Theory of Atoms in Molecules) analysis of the electron and electron spin densities of the investigated compounds, along with an energy decomposition analysis of the initial and reduced forms to unearth key parameters governing voltage ranges and tunability. The original contribution of Dr. Carlo Gatti relates particularly this aspect of the research

#### Recent examples:

- **Engineering of unsubstituted quinoid-like frameworks enabling a 2 V vs  $\text{Li}^+/\text{Li}$  redox voltage tunability and related derivatives**, D. Tomerini, C. Gatti and C. Frayret PCCP, 17, 8604-8608 (2015).

A criterion for redox voltage tuning (0.96–2.96 V vs.  $\text{Li}^+/\text{Li}$ ) has been derived from DFT calculations on quinoneazine and analogues (C/O replacing N). As rationalized through spin–charge distributions and energetic criteria, high–low voltage implying a bridge with delocalized–localized bond nature *mainly originates from ring stabilization*.

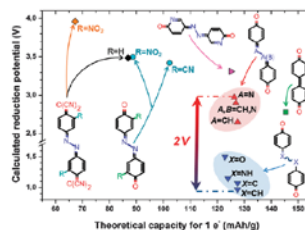
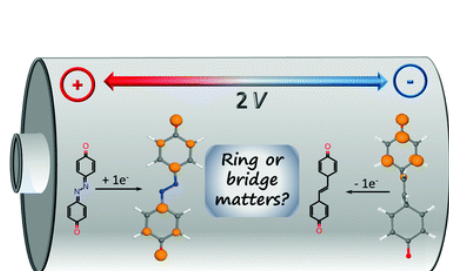
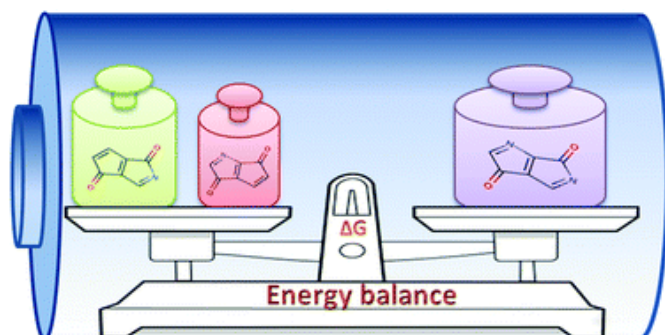


Fig. 2 Calculated reduction potential (in V vs.  $\text{Li}^+/\text{Li}$ ) as a function of the capacity for a one-electron process.

- **Playing with isomerism and N substitution in pentalenedione derivatives for organic electrode batteries: how high are the stakes?** D. Tomerini, C. Gatti and C. Frayret PCCP, 18, 2442-2448, (2016)

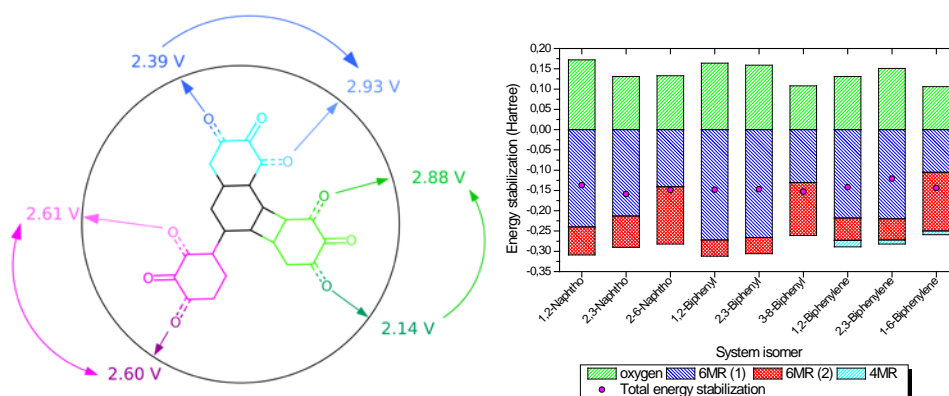
Isomerism and N single/double substitution for C on the parent backbone provides a series of compounds within the range of 2.2 – 3.6 V vs.  $\text{Li}^+/\text{Li}$ . Beyond learning gained for this peculiar family, these results may have exciting implications for future design strategies.

The incidence of double N substitution alone follows an almost additive rule based on the combined actions of the composing single N substitutions. Few exceptions to the rule are however, also observed and rationalized.



- **Electronic structure and energy decomposition analyses as a tool to interpret the redox potential ranking of Naphtho-, Biphenyl- and Biphenylene-quinone isomers, D. Tomerini, O. Politano, C. Gatti\* and C. Frayret\*, *Physical Chemistry Chemical Physics*, 18, 26651-26660 (2016)**

By calling to modelling approaches we have performed a comparative study on the redox property of various Naphtho-, Biphenyl- and Biphenylene-quinone isomers. These different compounds exhibit as a whole a redox potential range between 2.09 and 2.90 V vs. Li<sup>+</sup>/Li. A specific methodology was used to decrypt the interplay among isomerism, aromaticity and antiaromaticity modifications and the stabilization/destabilization effects due to other molecular components on this key electrochemical feature for electrode materials of batteries. In particular, energy decomposition analysis, within the Quantum Theory of Atoms in Molecules, along with the electron and electron spin population changes upon reduction nicely rationalise the observed potential trends. While 1,2- and 2,3- isomers show the highest/lowest redox potential in the Biphenylene-quinone series, a reverse trend is observed for the Naphtho-quinone, the compound having the two carbonyl groups on distinct rings being characterized by an intermediate value in both cases. There is instead almost no differentiation between 1,2 and 2,3 isomers for the Biphenyl-quinone family.



### Most important scientific discoveries/achievements:

1. Implementation of Quantum Theory of Atoms in Molecules (Bader's theory) for periodic systems (including crystals) from ab-initio computations
2. Contributions to the implementation of Quantum Theory of Atoms in Molecules (Bader's theory) for periodic systems (including crystals) from X-ray derived charge densities
3. Packing effects in crystals from electron density topology
4. Molecular dipole moment enhancement in crystals
5. Non-nuclear electron density maxima (non-nuclear attractors) in metallic clusters, metals and F-centers
6. Experimental vs theoretical topological properties of the electron density in crystals: comparisons and assessment of multipolar model bias
7. Source function for the electron density, the electron spin density and the electrostatic potential density: proposal, theory and applications
8. Electron Localization Function description of metallic bond

9. Discovery and characterization of the first ionic phase for an element (gamma Boron) and of the first stable compound of He (Na<sub>2</sub>He)
10. Phase diagram for Boron
11. Interpretation of Quantum Theory of Atoms in Molecules: Bond paths as privileged exchange channels
12. Thermoelectric materials: effect of actual geometric/compositional structure on Seebeck coefficient. Thermoelectric materials (TE): bonding vs properties relationships in most promising new TMs.
13. Relationships between the physical properties of chalcogenide phase change materials and their chemical bonding features ("metavalent" bonding)

## The 15 most cited papers, ISI-WEB of Science, as of December 2020 (in parenthesis the datum from Google Scholar)

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1. **618 (831) times** A. R. Oganov, J. Chen, **C. Gatti**, Yanzhang Ma, Yanming Ma, C. W. Glass, Z. Liu, T. Yu, O. O. Kurakevych, V. L. Solozhenko, "Ionic high-pressure form of elemental boron", *Nature* **457**, 863-868 (2009)
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3. **478 (567) times**, **C. Gatti**, 'Chemical bonding in crystals: new directions', invited review, *Zeitschrift für Kristallographie*, **220**, 399-457 (2005).
4. **248 (296) times** A. Martín Pendás, E. Francisco, M. A. Blanco and **C. Gatti**, "Bond paths as privileged exchange channels", *Chemistry an European Journal*, **13**, 9362-9371, (2007)
5. **241 (323) times** M. S. Toprak, C. Stiewe, D. Platzek, S. Williams, L. Bertini, E. Müller, **C. Gatti**, Y. Zhang, M. Rowe, M. Muhammed, 'The impact of Nanostructuring on the Thermal Conductivity of Thermoelectric CoSb<sub>3</sub>', *Adv. Funct. Mater.* **14**, 1189-1196 (2004).
6. **215 (247) times**, R. F. W. Bader, A. Larouche, **C. Gatti**, M.T. Carroll, P.J. MacDougall, K. Wiberg, 'Properties of atoms in molecules: Dipole moments and transferability of properties', *J. Chem. Phys.* **87**, 1142-1152 (1987).
7. **194 (233) times** R.F.W. Bader, **C. Gatti**, 'A Green's function for the density', *Chem. Phys. Lett.* **287**, 233-238 (1998) (important as it introduces the Source Function descriptor)
8. **176 (227) times** X. Dong, A. R. Oganov, A. F. Goncharov, E. Stavrou, S. Lobanov, G. Saleh, G.-R. Qian, Q. Zhu, **C. Gatti**, V.L. Deringer, R. Dronskowski, X.-F. Zhou, V. Prakapenka, Z. Konôpková, I. Popov, A. I. Boldyrev and H.-T. Wang "Stable Compound of Helium and Sodium at High Pressure", *Nature Chemistry*, **9**, 440-445 (2017)
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10. **159 (195) times**, A.Volkov, Y. Abramov, P. Coppens\* and **C. Gatti**, 'On the origin of topological differences between experimental and theoretical crystal charge densities', *Acta Cryst.* **A56**, 332-339 (2000).
11. **159 (188) times**, B. Silvi\*, **C. Gatti**, 'Direct Space Representation of the Metallic Bond', *J. Phys. Chem. A*, **104**, 947-953, (2000)
12. **153 (188) times**, W.L. Cao, **C. Gatti**, P.J. MacDougall, R.F.W. Bader, 'On the presence of Non-Nuclear Attractors in the Charge Distributions of Li and Na clusters', *Chem. Phys. Lett.* **141**, 380-385 (1987).

13. **147 (179) times**, C. Gatti, P. Fantucci, G. Pacchioni, 'Charge density topological study of bonding in lithium clusters', Theor. Chim. Acta **72**, 433-458 (1987).
14. **146 (178) times** F. Cargnoni, E. Nishibori, P. Rabiller, L. Bertini, G. J. Snyder, M. Christensen, C. Gatti\*, B. B. Iversen\*, 'Interstitial Zn atoms Do the Trick in Thermoelectric Zinc Antimonide, Zn<sub>4</sub>Sb<sub>3</sub>: A combined Maximum Entropy Method X-ray Electron Density and Ab Initio Electronic Structure Study', Chem. Eur. J. **10**, 3861-3870 (2004)
15. **145 (169) times** C. Gatti\*, F. Cargnoni, L. Bertini, 'Chemical Information from the Source Function', J. Comput. Chem. **24**, 422-436, (2003)

## Internationally distributed scientific software

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- **TOPOND-98**: An electron density topological program for systems periodic in 0-3 dimensions, User's Manual CNR-ISTM, Milan 1999; It is described in J. Chem. Phys. 101 (1994) 10686-10696. The code implements the Quantum Theory of Atoms in Molecules (QTAIM) for periodic systems (molecules, polymers, slabs and crystal). This code has been first interfaced to CRYSTAL-98, a code for performing ab-initio calculations on periodic systems, including crystals and then to the following releases of CRYSTAL, up to CRYSTAL-09.
- **TOPOND14** in CRYSTAL-14 and in CRYSTAL-17 releases. It is the original TOPOND code, properly modified and incorporated into CRYSTAL code (<http://www.crystal.unito.it/index.php>) releases since CRYSTAL-14, in collaboration with S. Casassa. TOPOND has become one of the possible properties evaluated from the *properties* section of the CRYSTAL code (C. Gatti and S. Casassa, TOPOND14, User's Manual, 2014, <http://www.crystal.unito.it/topond/topond.pdf>)
- **TOPXD** (C. Gatti and A. Volkov): Topological analysis program for experimental static electron density based on Hansen-Coppens multipole formalism, (Volkov, A.; Gatti, C.; Abramov, Yu.; Coppens, P. Acta Cryst. A.2000, 56, 252). The code interfaces the TOPOND-98 code with the XD package, a program for the multipolar analysis of X-ray diffraction intensities (see Volkov, A.; Gatti, C.; Abramov, Yu.; Coppens, P. Acta Cryst. A.2000, 56, 252 and <http://harker.chem.buffalo.edu/public/topxd/>)
- **XD2006** (Volkov, A.; Macchi, P.; Farrugia, L. J.; Gatti, C.; Mallinson, P.; Richter, T.; Koritsanszky, T.) - A Computer Program Package for Multipole Refinement, Topological Analysis of Charge Densities and Evaluation of Intermolecular Energies from Experimental and Theoretical Structure Factors Official site: <http://xd.chem.buffalo.edu/>
- **NCI-Milano** (G. Saleh, L. Lo Presti, C. Gatti, D. Ceresoli, *NCImilano: an Electron Density-based code for the study of Non-Covalent Interactions*, J. Appl Cryst 46, 1513-1517 (2013). NCI-Milano, is a Fortran90 code for applying the reduced density gradient (RDG) descriptor to a real-space study of noncovalent interactions. Designed specifically for the X-ray charge density community. Enables also plotting of energy densities over RDG isosurfaces.

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11. **C. Gatti\***, A. M. Orlando, E. Monza and L. Lo Presti, *Exploring Chemistry through the Source Function for the Electron and the Electron Spin Densities* chapter 5, pp 101-129 in Applications of Topological Methods in Molecular Chemistry, Remi Chauvin, Christine Lepetit, Bernard Silvi and Esmail Alikhani (Eds), Challenges and Advances in Computational Chemistry and Physics, **22**, Springer International Publishing Switzerland, (2016), DOI 10.1007/978-3-319-29022-5\_5
12. **C. Gatti\*** and A. Forni, 'Revealing the intermolecular bonds in molecular crystals through charge density methods', chapter 18, pages 617-672 in Intermolecular Interactions in Crystals: Fundamentals of Crystal Engineering, Juan J. Novoa editor, Royal Society of Chemistry, (2017)
13. G. Saleh, D. Ceresoli, G. Macetti and **C. Gatti\***, "Chemical Bonding Investigations for Materials", chapter 5 of *Computational Materials Discovery*, A.R. Oganov, G. Saleh, A.G. Kvashnin Eds, Royal Society of Chemistry, Pages 117 – 175, (2018) <http://dx.doi.org/10.1039/978178801012>
14. Á. M. Pendás, **C. Gatti**, *Quantum theory of atoms in molecules and the AIMAll software* chapter 3, pages 43-74, in *Complementary Bonding Analysis*, Simon Grabowsky Ed., De Gruyter (2021) <https://doi.org/10.1515/9783110660074-003>

## Invited lectures at International Conferences and Workshops

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1. **C. Gatti**: 'The quantum theory of atoms in molecules and the description of the chemical concepts', plenary lecture at the meeting *Progress in molecular structure analysis*, in honour of Prof. M. Simonetta, Como 8-9 gennaio 1987.
2. **C. Gatti**: 'Topological features of electron density in clusters and periodic systems', at the workshop on *Periodic vs Cluster ab-initio Treatment of Condensed Systems*, CECAM workshop Orsay, October 10-18 1991.
3. **C. Gatti**: 'Topologia della densita' elettronica in sistemi periodici', plenary lecture, XX Congreso del Quimicos Teoricos de los paises de Expresion Latina, Merida (Venezuela), 12-17 ottobre, 1992.
4. **C. Gatti**: 'Electron density and packing effects', 45' minutes talk at Gordon Research Conference on *Electron Distribution and Chemical Bonding*, Plymouth State College, N. Hampshire, USA, July 2-7, 1995.
5. **C. Gatti**: 'The electron density topology and the characterization of atomic interactions in molecules and crystals', Aminoff Symposium on *Electron Density and Chemical Bonding*, The Royal Swedish Academy of Sciences, Stockholm, Sweden, 25 march 1996 (on the occasion of the Aminoff Prize award to Prof. Philip Coppens) .
6. **C. Gatti**: 'Implementation of the Quantum Theory of Atoms in Molecules to Periodic Systems', 10th Seminar on Computational Methods in Quantum Chemistry, Strasbourg, September 4-6, 1996
7. **C. Gatti**: 'Playing with the Quantum Theory of Atoms in Molecules in the solid state', Symposium on the occasion of the 65<sup>th</sup> birthday of R.F.W. Bader, McMaster University, Hamilton, Ontario, CANADA, October 18-20, 1996.
8. **C. Gatti**: 'Interaction densities and energies using the theory of Atoms in Molecules and Crystals', Sagamore XII on *Charge, Spin and Momentum Density*, July 27-August 1, 1997, Waskesiu, Saskatchewan, Canada.
9. **C. Gatti**, G.K.H. Madsen and E. May " Weak cooperative electron-electron or molecule-molecule interactions in inorganic and organic crystals. A Quantum Theory of Atoms in Crystals approach", plenary lecture (C. Gatti) at the 2nd European Charge Density Meeting, Sitges (Barcelona, Spain) 30th September-2 October 1999.
10. **C. Gatti** " *Exploiting the theoretical electron and spin densities*", 30' lecture in the microsymposium "New developments in Charge, Spin and Momentum Densities", XIXth European Crystallographic Meeting, ECM 19, Nancy, France, 25<sup>th</sup>-31<sup>st</sup> August 2000, pag. 20 Abstracts.

11. **C. Gatti**: "The topology of charge density in crystals", Workshop on X-ray Charge Density Analysis and the XD Programming package, Buffalo, SUNY, NY, 13-17 May 2003.
12. **C. Gatti** "Search of critical points of the electron density", 30' short lecture at Workshop on X-ray Charge Density Analysis and the XD Programming package, Buffalo, SUNY, NY, 13-17 May 2003.
13. **C. Gatti** "Interpretation of results. Characterization of intermolecular interactions in crystals", short 30' lecture at Workshop on X-ray Charge Density Analysis and the XD Programming package, Buffalo, SUNY, NY, 13-17 May 2003.
14. **C. Gatti**: "Chemical Information from the Source Function", 40' lecture at European Science Foundation Exploratory Workshop ESF/PESC, Sandbjerg Estate, Sønderborg, Denmark, 26-29 June 2003.
15. P. Macchi, **C. Gatti** "XD: From Multipolar Model Refinement to Complete Topological Analysis. A description of the new features", joint (50% Macchi, 50% Gatti) 45' lecture at ECDM-III, 3<sup>rd</sup> European Charge Density Meeting, Sandbjerg Estate, Sønderborg, Denmark, 24-26 June 2003.
16. **C. Gatti** , "Chemical Information from the Source Function", 30' lecture, Sagamore XIV Meeting, on Charge, Spin and Momentum Densities, Broome, Kimberley, Australia, 13-18 August 2003.
17. **C. Gatti** , "Nano-engineering and nano-structuring of novel thermoelectric materials: the computational approach", invited 30' lecture at Workshop in Nanotechnology and Nanoscience, Ministry of Science and Technology, Brazil - European Commission, São Paulo, Sp, Brazil, December 13-15, 2004.
19. **C. Gatti**, L. Bertini, F. Cargnoni, (conference delivered by C. Gatti) 25' lecture on "Beyond  $\nabla^2\rho_b$  : chemical bond analysis using the local form of the source function", XX Congress of the IUCr, Florence 23-31 August 2005.
20. **C. Gatti**, D. Lasi (conference delivered by C. Gatti) : " Unambiguous electron population analysis from the electron density observable?", 30' minutes lecture at 4th European Charge Density Meeting, Branderburg/Havel (Germany), 26-29 January 2006.
21. **C. Gatti**, D. Lasi (conference delivered by C. Gatti) : 40' minutes lecture " The Source Function and the Nature of the Chemical Bond", VII Girona Seminar on the Nature of the Chemical Bond, July 10-13 2006, Girona, Spain.
22. **C. Gatti**: "Chemical bonding in crystals: new directions", 35' minutes lecture at Sagamore XV Conference, Bosworth Hall Hotel, Warwickshire, UK, 13-18 August 2006.
23. **C. Gatti**, D. Lasi (invited presentation and discussion held by C. Gatti) : "Source Function description of metal-metal bonding in d-block organometallic compounds", Faraday Discussion 135: Chemical Concepts from Quantum Mechanics, 4-6 September 2006, Manchester, UK.
24. **C. Gatti**, "What the Source Function tells Us about Chemical Bonding", 25' lecture at Bunsen-Kolloquium on "Chemical Bonding in Position, Momentum , and Phase Space, February 5-6, 2007, Universität Konstanz, Konstanz, Germany.
25. **C. Gatti**, " The Quantum Theory of Atoms in Molecules: bond paths, chemical bonds and chemical binding", 50' lecture at Workshop on XD2006 program package: Advanced methods in X-Ray Charge Density Analysis: Extracting properties from a Multipole Refinement, September 3-6 2007, Martina Franca (Italy).
26. **C. Gatti**, "The Source Function", 45' lecture at Workshop on XD2006 program package: Advanced methods in X-Ray Charge Density Analysis: Extracting properties from a Multipole Refinement, September 3-6 2007, Martina Franca (Italy).
27. **C. Gatti**, A.R Oganov, J. Chen, Y. Ma, " How and why elemental boron undergoes self charge transfer between 19 and 89 GPa, 30' (given by C. Gatti) at XXI Congress of the International Union of Crystallography (IUCr) , Osaka, Japan, 23-31 August 2008. Published in Acta Cryst. **A64** C70 (2008)

28. **C. Gatti**, " How and why elemental boron undergoes self charge transfer between 19 and 89 GPa, 30' lecture at *Ab initio simulation of crystalline solids: history and prospects, workshop in honour of Prof. Cesare Pisani*, Torino, September 8-9 2008.
29. **C. Gatti**, " Self-charge transfer in an element: the *ionic* high pressure form of Boron", 55' minute lecture at workshop on *Touching Chemical Bonds without experiments*, Facultad de Quimica, Universidad de Oviedo, Oviedo (Spain), 18 December 2008
30. **C. Gatti**, " Self-charge transfer in an element: the *ionic* high pressure form of Boron", 40' minute lecture at Gordon Research Conference on Solid State Chemistry, August 30- September 4, Magdalen College, Oxford, UK, 2009
31. **C. Gatti**, " Topologie de la densité électronique et liaison chimique. Description détaillée de la théorie de Bader", 120' lecture at Int. workshop on the refinement and analysis of the electron density obtained from high resolution X-ray diffraction, 28-30 October 2009, Marrakech, Maroc
32. **C. Gatti** "Insights from theory on challenging problems in chemistry" 30' lecture on the occasion of the Center for Materials Crystallography Kick-off Meeting, 14-15 April 2010, *Danish National Research Foundation*, Department of Chemistry and iNANO, University of Aarhus (Denmark)
33. **C. Gatti** "Update from Milano" 30' lecture on the occasion of the First review meeting, Center for Materials Crystallography, 2 November 2010, *Danish National Research Foundation*, Department of Chemistry and iNANO, University of Aarhus (Denmark)
34. **C. Gatti**, A.R. Oganov, V.L. Solozhenko, "Structure, bonding and Charge Transfer in  $\gamma$ -B<sub>28</sub> " ISBB 2011 – 17<sup>th</sup> International Symposium on Boron, Borides and Related Materials, September 11-17, 2011 Istanbul, Turkey (note: C. Gatti invited talk, prepared, but not delivered at the very last moment because of my father-in-law death)
35. **C. Gatti**, "Revealing electron delocalization through the Source Function", X-ray and Neutron Scattering for Solving Structures and Modelling Charge Densities: the last 40 years. A colloquium in honour of Pierre J. Becker, Chateau de Sept Tours, Courcelles de Touraine, France, September 16-17, 2011
36. **C. Gatti**, "Making experiment and theory talking together : electron delocalization effects and non covalent interactions detection *via* the Source Function and the Reduced Density Gradient", Sagamore XVII Conference on Electron Charge Spin and Momentum Densities, Kitayuzawa, Hokkaido, Japan, July 15-20, 2012.
37. **C. Gatti**, G. Saleh, L. Lo Presti "Using X-ray derived Charge Densities to detect electron delocalization effects and non-covalent interactions", Sixth European Charge Density Meeting, ECDM-6, Strbske pleso, Slovakia, September 15-20 (2012)
38. **C. Gatti**, "Challenging chemical concepts through charge density" Symposium on Charge Density in Crystals, invited plenary lectures given by the 2013 Aminoff Prize recipients, 2 April 2013, Ångström Laboratory, Uppsala University, Uppsala, Sweden
39. **C. Gatti**, "Challenging chemical concepts through charge density" Aminoff Prize Lectures 2013, 4 April 2013, Stockholm University, Stockholm, Sweden
40. **C. Gatti**, "Challenging chemical concepts through charge density" Aminoff Prize Lectures 2013 (in collaboration with the Royal Swedish Academy of Sciences the two prize winners have repeated their Aminoff Lectures at Aarhus University), 8 April 2013, Dept. of Chemistry, Aarhus University, Aarhus, Denmark
41. **C. Gatti** "Spin polarization studied through the spin density Source Function", invited plenary lecture at Gordon Conference on Electron Distribution and Chemical Bonding, June 2-7, 2013, Les Diablerets Conference Center Les Diablerets, Switzerland
42. **C. Gatti** "Challenging chemical concepts through charge density" Workshop in Solid State Quantum Chemistry" in honour of Prof. Cesare Pisani, Torino (Italy), 6-7 September 2013

43. **C. Gatti** "Chemical bonding in crystals: charge density and beyond", invited plenary lecture at MISSCA 2013, Meeting of the Italian, Spanish and Swiss Crystallographic Associations, September 9<sup>th</sup>-12<sup>th</sup>, 2013, Villa Olmo, Como, Italy
44. **C. Gatti** "New descriptors for an "unbiased" and chemically insightful comparison of ab-initio and X-ray derived charge densities", invited 40' lecture at *Natta's Seeds Grow, From the crystallography and modelling of stereoregular polymers to the challenges of complex systems*, International symposium on occasion of the 50<sup>th</sup> anniversary of the award of the Nobel Prize for Chemistry to Giulio Natta and Ziegler, Politecnico di Milano, 21-22 November 2013
45. **C. Gatti**, "Step by step understanding of the energetics of the BH<sub>4</sub><sup>-</sup> rotation in MBH<sub>4</sub> crystals (M=Li, Na, K, Rb, Cs)", 25' invited lecture, Center for Materials Crystallography, 8<sup>th</sup> Workshop, 27<sup>th</sup> March 2014, Institute of Inorganic Chemistry, Georg-August-University Göttingen, Germany
46. **C. Gatti**, A. M. Orlando, L. Lo Presti, "Insights on spin-polarization *via* the spin density Source Function", invited oral lecture, delivered by Carlo Gatti, XXIII Congress of the International Union of Crystallography (IUCr), Montréal, Canada, August 5-12, 2014
47. **C. Gatti**, "The electron spin density Source Function: conceptual progresses", CMC Annual Meeting, 3-4 June 2015, Dept. of Chemistry, Aarhus University, Aarhus, Denmark
48. **C. Gatti**, invited 1hr lecture "Solving chemistry puzzles in molecules and crystals through electron and electron spin density analyses", DN-NSM 2015, Discovery of Novel Nanoparticles, Surfaces and bulk Materials, 9th USPEX workshop on Crystal Structure Prediction and Materials Discovery, Poitiers (France), 25-30 June 2015
49. **C. Gatti**, "Solving chemistry puzzles in molecules and crystals through electron and electron spin density analyses", keynote lecture at 29<sup>th</sup> European Crystallographic Meeting, ECM-29, 29th European crystallographic meeting, August 23-28, 2015, Rovinj, Croatia
50. **C. Gatti**, "*Chemical insights from experiment and theory using the Source Function for the electron and the electron spin densities*", invited 50' plenary lecture at "Frontiers in Computational Chemistry 2016, international congress on occasion of the School of Chemistry celebrating its first century at National Autonomous University of Mexico (UNAM) in Mexico City, August 24-25, 2016, Mexico. <http://www.iquimica.unam.mx/dfq/>
51. **C. Gatti**, "*Talking to Philip: a truly special, training and enjoyable experience! And some words on the Source Function for the Electron Spin Density*" invited 40' plenary lecture in "Advancing Structural Science: Pushing the limits of X-ray Crystallography, a symposium in honour of the scientific achievements of Professor Philip Coppens, 22<sup>nd</sup> October 2016, Dept. of Chemistry, University of Buffalo, The State University of New York, Buffalo, NY, USA
52. **C. Gatti**, "*The Source Function for the Electron Spin Density*", invited 45' lecture, ChemBond 2016, Chemical Bonding in Position Space, November 27-December 1, 2016, Max Planck Institute für Chemische Physik Fester Stoffe, Dresden, Germany Dresden
53. **C. Gatti**, "What is Quantum Crystallography?" CECAM Discussion Meeting on Quantum Crystallography: Current Developments and Future Perspectives, Nancy, 19-20 June 2017
54. **C. Gatti**, "Insights on spin density delocalization/polarization mechanisms through the Source Function", 24th Congress and General Assembly of the IUCr, 21-28 August 2017, Hyderabad, India
55. **C. Gatti**, "Insights on spin density delocalization/polarization mechanisms through the Source Function: general aspects", CMC annual meeting, 2-3 October 2017, Aarhus, Denmark
56. **C. Gatti** (presenter) and G. Macetti, 20' minutes talk on "Quantum Crystallography put into action: assessing the accuracy of and getting insights on the electron spin densities" delivered as a part of the Round Table on the *Future of Quantum Crystallography*, 52th Crystallographic Course *Quantum Crystallography*, Erice, Centro Ettore Majorana (Trapani, Sicily), Italy, 1-10 June 2018



57. **C. Gatti** (presenter), G. Macetti and L. Lo Presti, 20' invited talk on Getting more physical and chemical insight into electron spin density distributions and their accuracies, ESB2, Second European Symposium on Chemical Bonding, Oviedo, 3-7 September (2018)
58. **C. Gatti**, 30' invited talk on *Exporting charge density and chemical bonding know-how elsewhere*, First International Charge Density Meeting, 21-26 luglio 2019, Goettingen, Germania
59. **C. Gatti**, invited plenary lecture (40') on *Novel paths for the study of spin polarized systems and phase change materials*, Chitel/Quitel 2019, Montreal, Canada, 25-31 Agosto 2019
60. **C. Gatti** (presenter), Paola Peluso, 20' invited talk on Non covalent interactions as viewed through the Source Function Descriptor, 1st International Conference on Non Covalent Interaction, 2-6 settembre 2019, Lisbona, Portogallo
61. **C. Gatti**, "Electron Spin Density Topology", first opening invited lecture at CECAM *Second discussion Meeting on Quantum Crystallography: expectations and reality*, Flagship Workshop, September 9, 2021 - September 12, 2021,
62. **C. Gatti**, "Wavefunction analyses in real space using Quantum Chemical Topological Methods", MSCC2021, Ab initio modelling in Solid State Chemistry, September 20-24 2021, Imperial College, London, UK
63. **C. Gatti**, "Real space approaches to chemical bonding and physical properties", invited plenary lecture in the dedicated session "Geochemical thermodynamics: a Tribute to Giulio Ottonello" within the 1st Italian Geochemical Society Congress "From theoretical to applied geochemistry", 15-18 February 2022, Palazzo Rosso, Genova.

## Chairing of International conferences/microsymposia

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1. **C. Gatti, chair (co-chair R. Stewart, USA)** Microsymposium Topology II, XVII International Union of Crystallography Congress, Seattle, USA, 8-17, 1996.
2. **C. Gatti, co-chair (chair F.K. Larsen, DK)** Microsymposium "New developments in Charge, Spin and Momentum Densities", XIXth European Crystallographic Meeting, ECM 19, Nancy, France, 25<sup>th</sup>-31<sup>st</sup> August 2000.
3. **C. Gatti, co-chair (chair P. Mallinson, UK)** Microsymposium "Wavefunctions and properties from experiment", XXth European Crystallographic Meeting, ECM 20, Krakow, Poland, 25<sup>th</sup>-31<sup>st</sup> August 2001.
4. **C. Gatti, chair (co-chair M. Cooper, UK)** Microsymposium "Molecular and Crystal Properties from Charge and Spin Densities", 9 august 2002, IUCr XIX, 6-15 August 2002, Geneve, Switzerland.
5. **C. Gatti, co-chair (chair P. Becker, France)** microsymposium "The synergy of experiment and theory in studies of charge, spin and momentum densities", ECM-21, Durban, South Africa, 24-29 August 2003
6. **C. Gatti, co-chair (chair John Spence, USA)** of the **Gordon Research Conference** on "Electron Distribution and Chemical Bonding. The Chemical Bond: Densities and Dynamics", Mount Holyoke College, South Hadley, Massachusetts (USA), July 4-9, 2004.
7. **C. Gatti chair (co-chair Dylan Jayatilaka, Australia)** of the **Gordon Research Conference** on "Electron Distribution and Chemical Bonding. The Chemical Bond: Densities and Dynamics", Mount Holyoke College, South Hadley, Massachusetts (USA), July 1-6, 2007.
8. **C. Gatti, chair** of the session on the "Interaction between Theory and Experiment", Sagamore XVI, Santa Fe, New Mexico, USA, August 2-7, 2009.

9. **Invited Chair** (but with no choice of the speakers) of the 22 June 2010 afternoon session at the “20 Years of ELF” Workshop, a workshop to celebrate ELF's (Electron Localization Function) 20th birthday, and to honor the contribution of Bernard Silvi who is retiring, 20-24 June 2010, Paris, France.
10. **Invited Chair** for the keynote lecture (K21) of B.B. Iversen on *Charge Densities and Materials Crystallography*, at XXII IUCr Congress and General Assembly of the International Union of Crystallography, Madrid, Spain, 22-30 August, 2011
11. **Invited Session Chair** (but with no choice of the speakers) at ISBB 2011 – 17<sup>th</sup> International Symposium on Boron, Borides and Related Materials, Session on New Materials and Preparation, September 11-17, 2011 Istanbul, Turkey
12. **Invited Session Chair** (with an introductory talk of about 5 minutes on the contribution of Pierre Becker to the field of the session but with no choice of the speakers) at *X-ray and Neutron Scattering for Solving Structures and Modelling Charge Densities: the last 40 years. A colloquium in honour of Pierre J. Becker*, session on Charge Density and chemical bonding (experimental aspects). Chateau de Sept Tours, Courcelles de Touraine, France, September 16-17, 2011
13. **C. Gatti conference chair** of the Sagamore XVIII meeting on Charge, Spin and Momentum Densities, 7-12 June 2015, Santa Margherita di Pula, Italy
14. **C. Gatti**, Conference chair, along with Prof. Artem Oganov and Dr. Davide Ceresoli of the International Symposium on Material Design & the 11<sup>th</sup> USPEX workshop, villa Monastero, Varenna, Lake Como, Italy, 5-9 June 2016.
15. **C. Gatti**, Chair of the Round Table on *Future Perspectives and a Vision for Quantum Crystallography*, CECAM meeting CECAM Discussion Meeting on Quantum Crystallography: Current Developments and Future Perspectives, Nancy, 19-20 June 2017
16. **C. Gatti**, Chair of the Award Lecture session of the International Miguel Blanco Prize 2018 at the congress Sagamore XIX on Quantum Crystallography - Charge, Spin and Momentum Densities, 8-13 July 2018, Halifax, Canada, <http://www.sagamore2018.ca/award-lectures/>
17. **C. Gatti**, Invited 4<sup>th</sup> session chair at CECAM *Second discussion Meeting on Quantum Crystallography: expectations and reality*, Flagship Workshop, September 9, 2021 - September 12, 2021,

## Discussion leader at Gordon Research Conferences or at Other International Conferences

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1. **C. Gatti, discussion leader** (substituting Richard Bader) of session on *Topology* at the Gordon Research Conference on *Electron Distribution and Chemical Bonding*, Queen's College, Oxford, UK, August 30, September 4, 1998.
2. **C. Gatti, discussion leader** of the session *New Developments in Topological Analysis* at the Gordon Research Conference on *Electron Distribution and Chemical Bonding*, Mount Holyoke College, Bradley, MA (USA) July 8-13, 2001.
3. **C. Gatti, discussion leader** (substituting David J. Singh) of the session *Thermoelectrics* at the Gordon Research Conference on *Electron Distribution and Chemical Bonding*, Mount Holyoke College, Bradley, MA (USA) July 4-9, 2004.
4. **C. Gatti, discussion leader of the session** *Chemical Bonds under Extreme Conditions* at the Gordon Research Conference on *Electron Distribution and Chemical Bonding*, Mount Holyoke College, Bradley, MA (USA) July 11-16, 2010
5. **C. Gatti**, Discussion Leader of the Round Table on the science of Quantum Crystallography at the congress Sagamore XIX on Quantum Crystallography - Charge, Spin and Momentum Densities, 8-13 July 2018, Halifax, Canada, <http://www.sagamore2018.ca/>

## Invited lectures at National Conferences and Workshops

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1. **C. Gatti:** 'Analisi topologica della densità elettronica in sistemi periodici: il programma TOPOND', 20' lecture al Workshop *Esame comparativo di vari metodi di calcolo della struttura elettronica molecolare*, XXVIII Congresso Nazionale della Divisione di Chimica Fisica della S.C.I., Pisa 10-14 febbraio 1997
2. **C. Gatti** "Implementation of the Quantum Theory of Atoms in Molecules to Periodic Systems : the TOPOND code", 25' lecture at workshop on *Metodologie e Algoritmi per Sistemi Complessi*, IV Convegno *Sistemi Complessi: Struttura, Proprietà, Reattività e Dinamica*, 16-18 giugno, 1999, Varenna, Villa Monastero, Lecco, Italia.
3. **C. Gatti** "Nature and Function of CH...O interactions in crystals from their experimental and theoretical charge densities ", 30' lecture at XXX Congresso Nazionale AIC, Martina Franca (Taranto), 19-22 settembre 2000, pag. 60 Abstracts.
4. **C. Gatti:** "Chemical Information from Electron Densities and Wavefunctions", invited plenary lecture , PCEC 2002, Joint Meeting of the Physical Chemistry and Electrochemistry Divisions of the Italian Chemical Society, XXXII Italian Meeting of Physical Chemistry Italian Electrochemistry Days 2002, Ferrara, Italy, June 23-28, 2002.
5. **C. Gatti**, "Revealing electron delocalization through the Source Function", primo Congresso della Divisione di Chimica Teorica e Computazionale della Società Chimica Italiana, Pisa, Italia, 22-23 Febbraio, 2012
6. **C. Gatti**, "Dati, modelli e calcolo in cristallografia" lecture 30' in occasione della cerimonia di apertura e presentazione della mostra "Cristalli! In UNIMI", Aula Magna, Università degli Studi di Milano, 12 giugno 2014, Milano, Italy
7. **C. Gatti**, "Quantum Theory of Atoms in Molecules: theoretical background" 1 hr invited lecture held on 30th June, in the multidisciplinary course offered by the Scuola di Dottorato di Ricerca on *Simulation of molecular systems for chemistry, materials and biology*, Politecnico di Milano Dottorati di Ricerca in Chimica Industriale e Ingegneria Chimica, Ingegneria dei Materiali e Bioingegneria 26 June – 30 June 2017, Polo di Lecco, Politecnico di Milano
8. **C. Gatti**, "Quantum Theory of Atoms in Molecules: examples of applications" 1 hr invited lecture held on 30th June, in the multidisciplinary course offered by the Scuola di Dottorato di Ricerca on *Simulation of molecular systems for chemistry, materials and biology*, Politecnico di Milano Dottorati di Ricerca in Chimica Industriale e Ingegneria Chimica, Ingegneria dei Materiali e Bioingegneria 26 June – 30 June 2017, Polo di Lecco, Politecnico di Milano
9. **C. Gatti**, 30' conferenza invitata su "Tavola periodica sotto pressione: una periodicità diversa ed una chimica esotica", in convegno su "La Tavola periodica ha 150 anni...ma non li dimostra", Istituto Lombardo Accademia di Scienze e Lettere, Milano - via Brera 28, Palazzo Brera – Sala delle Adunanze, 21 marzo 2019.

## Invited Seminars at International Institutions

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1. **C. Gatti:** ' A charge density description of the structural and chemical changes in tautomeric systems : applications to bridged annulenes and homoaromatic systems', seminario tenuto il 4 dicembre 1986 presso il Department of Chemistry, McMaster University, Hamilton, Ontario, Canada.
2. **C. Gatti:** 'Charge density topology in Periodical Systems : Experimental and Theoretical Results', seminario tenuto presso il Centro de Química, IVIC, Caracas, Venezuela, il 21 ottobre 1992.

3. **C. Gatti:** ' The electron density topology and the characterization of atomic interactions in molecules and crystals', Centre for Crystallographic Studies , Department of Chemistry, University of Copenhagen , Denmark, 29 marzo 1996.
4. **C. Gatti:** " Interaction energy and density in the water dimer. A Quantum Theory of Atoms in Molecules Insight on the Effect of BSSE", Centre for Crystallographic Studies, Dept. of Chemistry, Univ. of Copenhagen, Copenhagen, Danimarca, 10 dicembre 1997.
5. **C. Gatti:** " The Topond's tale", Department of Chemistry, University of Aarhus, DK-8000 Aarhus, Denmark, 27 e 28 May 1999 (two seminars).
6. **C. Gatti:** " Weak C-H...O Interactions and their Effect on the Electron Distribution in Molecular Crystals", November 19, 1999, *Foster Chemistry Colloquia*, The State University of New York at Buffalo, Department of Chemistry.
7. **C. Gatti:** " Electron density studies of Si surface formation, reconstruction and coverage", Informal workshop on *Les distributions d'électrons*, Ecole Central de Paris, 24 April, 2001 École Central de Paris, 24 aprile 2001.
8. **C. Gatti** "Chemical Information from the Source Function", LCM<sup>3</sup>B, Laboratoire de Cristallographie et Modelisation des Materiaux Mineraux et Biologiques, UMR, CNRS 7036, Université Henri Poincaré, Nancy, France, 19 Gennaio 2007.
9. **C. Gatti** " Source Function description of metal-metal bonding in d-block organometallic compounds" , LCM<sup>3</sup>B, Laboratoire de Cristallographie et Modelisation des Materiaux Mineraux et Biologiques, UMR, CNRS 7036, Université Henri Poincaré, Nancy, France, 22 Gennaio 2007.
10. **C. Gatti** " Can an unambiguous electron population analysis be derived from the electron density observable?", LCM<sup>3</sup>B, Laboratoire de Cristallographie et Modelisation des Materiaux Mineraux et Biologiques, UMR, CNRS 7036, Université Henri Poincaré, Nancy, France, 30 Gennaio 2007.
11. **C. Gatti**, "Source Function analysis: use, scope, limitations", Institut für Organische Chemie, Universität Würzburg, Germany, 22 april 2009 (two seminars).
12. **C. Gatti**, "Aminoff Prize Summary", in front of the DNRF board, Third Annual Review of the Center for Materials Crystallography, April 9<sup>th</sup> 2013, Auditorium 6, Dept of Chemistry, Aarhus University, Aarhus, Denmark
13. **C. Gatti**, "Challenging chemical concepts through charge density", Seminari Chimici in occasione del premio Gregori Aminoff 2013, 16 aprile 2013, Università degli Studi di Milano, Milano
14. **C. Gatti**, "Solving (chemistry) puzzles in molecules and crystals through electron distributions descriptors", December 15<sup>th</sup> 2014, Université de Picardie - Jules Verne, Amiens, France
15. **C. Gatti**, " Quantum Theory of Atoms in Molecules: theoretical background", 90' seminar delivered at ISIS, 24 may 2016 morning, [STFC Rutherford Appleton Laboratory](#) , Oxford, UK.
16. **C. Gatti**, " QTAIM: examples of applications", 90' seminar delivered at ISIS, 24 may 2016 afternoon, [STFC Rutherford Appleton Laboratory](#) , Oxford, UK
17. **C. Gatti**. "Chemical Insights from experiment and theory using the Source Function for the electron and the electron spin densities", 20th January 2017, invited seminar at the Institut für Anorganische Chemie, RWTH Aachen University, Aachen, Germany
18. **C. Gatti** "From wavefunctions to chemical bond descriptors", invited 2hr seminar, in front of the PhD students in Physics, 20th July 2017, Institute of Physics (IA), RWTH Aachen University, Aachen, Germany.
19. **C. Gatti** " Do the peculiar physical properties of phase change materials entail unusual chemical bonding features?, Computational materials Science Seminar, 30<sup>th</sup> January 2020, Skolkovo Institute of Science and Technology, Moscow, Russia

20. **C. Gatti**, 60' seminar on "Wavefunction analyses in real space using Quantum Chemical Topological Methods", within the International Advance Materials Modeling course, 20 May 2021, Skolkovo Institute of Science and Technology, Moscow, Russia

## Invited Seminars at National Institutions

1. **C. Gatti**: 'Un potenziale modello non-empirico applicabile a calcoli Hartree-Fock molecolari per atomi della seconda e terza riga', Dipartimento di Chimica-Fisica, Università di Milano, febbraio 1979
2. **C. Gatti**: 'Un nuovo metodo di legame di valenza generalizzato ed autoconsistente per il calcolo di superfici di energia potenziale dello stato fondamentale e degli stati eccitati', Dipartimento di Chimica-Fisica, Università di Milano, marzo 1980.
3. **C. Gatti**: 'Tecniche di vettorializzazione di codici FORTRAN e loro ristrutturazione', Dipartimento di Chimica Fisica, Università di Milano, aprile 1984
4. **C. Gatti**: 'L'analisi topologica della densità di carica di molecole quale strumento per lo studio del legame chimico e delle proprietà degli atomi nelle molecole', seminario tenuto l'11 gennaio 1985 presso il Dipartimento di Chimica Industriale ed Ingegneria Chimica "Giulio Natta", Politecnico di Milano.
5. **C. Gatti**: 'Dai metodi quanto-meccanici NDO ai metodi ab-initio', seminario tenuto il 25 maggio 1990 nell'ambito della Scuola di Specializzazione in Sintesi Chimica "A. Quilico", presso il Dipartimento di Chimica, Politecnico di Milano.
6. **C. Gatti**: 'Sono le cariche di Bader effettivamente funzione della dimensione atomica? Popolazioni atomiche come valori di aspettazione di osservabili quantistiche', Università di Milano, Dipartimento di Chimica Fisica, giugno 1992.
7. **C. Gatti**: 'Teoria Quantistica degli atomi in molecole e solidi: caratterizzazione delle interazioni chimiche', Dipartimento di Fisica, Sezione Fisica dei Solidi e Nuovi Materiali, Università, 6 dicembre 1996, Milano.
8. **C. Gatti**: "Modellizzazione teorica ab-initio come supporto allo sviluppo di nuovi materiali termoelettrici", Politecnico di Torino, Dipartimento di Scienza dei Materiali e Ingegneria Chimica, 12 Ottobre 2007.
9. **C. Gatti**, "Boro elementare ad alta pressione: un "sale" costituito da un solo elemento", Istituto di Scienze e Tecnologie Molecolari, 20 febbraio 2009.
10. **C. Gatti**, "Challenging chemical concepts through charge density", Seminari Chimici in occasione del premio Gregori Aminoff 2013, 16 aprile 2013, Università degli Studi di Milano, Milano
11. **C. Gatti**, "Tavola periodica sotto pressione: una periodicità diversa ed una chimica esotica", seminario di 60', 15 aprile 2021, Università di Milano, Progetto Lauree Scientifiche, Appuntamenti con la Chimica, 2020/2021
12. **C. Gatti**, The Electrostatic Potential Source Function (EPSF) reconstruction: a valuable tool to study High-Performance Liquid Chromatography (HPLC) enantioseparations involving  $\sigma$  and  $\pi$ -holes as recognition sites, 20 aprile 2021, SCITEC DAYS, CNR-SCITEC, Milano
13. **C. Gatti**, "A scientific life at [CNR@UNIMI](https://www.cnr.it/en/unimi) (...and abroad)", 1 ottobre 2021, conferenza MeetMeOnChem, September 30<sup>th</sup> and October 1<sup>st</sup>, Chemistry dept, UNIMI

## Lectures as invited teacher in international schools/workshops

1. **C. Gatti:** 'Analisi della densità elettronica ed effetto dell'impaccamento cristallino', lezione (2 hr) tenuta nella scuola 1994 dell'Associazione Nazionale di Cristallografia *Acquisizione, valutazione ed utilizzo di dati diffrattometrici e strutturali in Cristallografia*, Perugia 3-7 ottobre 1994.
2. **C. Gatti :** 'Analisi Topologica della densità di carica', lezione ed esercitazione tenuta alla IV Scuola di Chimica Computazionale *Calcolo Quanto-Meccanico di Proprietà Chimico-Fisiche dei Materiali Cristallini*, Torino 19-24 settembre 1994.
3. **C. Gatti :** 'Electron density topological analysis in solids', lezione (1hr) ed esercitazioni (2hr) tenuta alla Network School of the Human Capital and Mobility Network on the *Developments and Applications of the Hartree-Fock method in Materials Science*, Turin (Italy), 17-27 September 1995.
4. **C. Gatti:** "Descrittori elettronici: Uso dei metodi quantomeccanici", lezione di 2.30 hrs tenuta il 5 giugno 1998 all'interno del corso *Uso di metodi computazionali per la determinazione di correlazioni struttura-attività*, Scuola di Specializzazione in Sintesi Chimica, Università di Milano.
5. **C. Gatti:** "Informazione chimica dall'analisi della densità elettronica" lezione all'interno del minicorso (coordinatore Carlo Gatti) *Metodi sperimentali e Teorici di Determinazione della densità di carica*, 18 settembre 2001, Parma (Italy).
6. **C. Gatti, A. Volkov** "Use of TOPXD for advanced users", tutorial held within Workshop on X-ray Charge Density Analysis and the XD Programming package, Buffalo, SUNY, NY, 13-17 May 2003.
7. **C. Gatti, A. Volkov** "Use of TOPXD for beginners", tutorial held within Workshop on X-ray Charge Density Analysis and the XD Programming package, Buffalo, SUNY, NY, 13-17 May 2003.
8. **C. Gatti, L. Lo Presti** "Evaluation of the source function in  $C_4F_6$  and  $Mn_2(CO)_{10}$ " tutorial held within Workshop on XD2006 program package: Advanced methods in X-Ray Charge Density Analysis: Extracting properties from a Multipole Refinement, September 3-6 2007, Martina Franca (Italy).
9. **C. Gatti,** "Topologie de la densité électronique et liaison chimique. Description détaillée de la théorie de Bader", 120' lecture at Int. workshop on the refinement and analysis of the electron density obtained from high resolution X-ray diffraction, 28-30 October 2009, Marrakech, Maroc
10. **C. Gatti,** "Topological analysis" 50' lecture at the Synchrotron Charge Density School, March 9-15, 2013, ChemMatCARS, Center for Advanced Radiation Sources, Argonne National Lab, The University of Chicago, Argonne-Chicago, Illinois, USA
11. **C. Gatti,** "The Source Function" 30' lecture at the Synchrotron Charge Density School, March 9-15, 2013, ChemMatCARS, Center for Advanced Radiation Sources, Argonne National Lab, The University of Chicago, Argonne-Chicago, Illinois, USA
12. **C. Gatti,** "Charge Density Topological Analysis in CRYSTAL", 30' invited lecture at the international school MSCC-2013, Ab-initio Modelling in Solid State Chemistry", Featuring CRYSTAL-13 and CRYSCOR13, Torino, 1-5 September 2013
13. **C. Gatti,** "About some features of the TOPOND code", International Symposium on Material design & the 11<sup>th</sup> USPEX Workshop, Villa Monastero, Varenna, Lake of Como, Italy, 5-9 June 2016.
14. **C. Gatti,** "Quantum Theory of Atoms in Molecules: theoretical background" 1 hr invited lecture held on 30th June, in the multidisciplinary course offered by the Scuola di Dottorato di Ricerca on *Simulation of molecular systems for chemistry, materials and biology*, Politecnico di Milano Dottorati di Ricerca in Chimica Industriale e Ingegneria Chimica, Ingegneria dei Materiali e Bioingegneria 26 June – 30 June 2017, Polo di Lecco, Politecnico di Milano
15. **C. Gatti,** "Quantum Theory of Atoms in Molecules: examples of applications" 1 hr invited lecture held on 30th June, in the multidisciplinary course offered by the Scuola di Dottorato di Ricerca on *Simulation of molecular systems for chemistry, materials and biology*, Politecnico di Milano, Dottorati di Ricerca in Chimica Industriale e Ingegneria Chimica, Ingegneria dei Materiali e Bioingegneria 26 June – 30 June 2017, Polo di Lecco, Politecnico di Milano



## List of papers on peer-reviewed International Congress Proceedings

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1. R. Bianchi, R. Destro, **C. Gatti**, F. Merati, 'A low-temperature (23K) study of L-alanine : topological properties of experimental and theoretical charge distributions, NATO ASI on *The application of charge density research to chemistry and drug design*, G.A. Jeffrey and J.F. Piniella (Eds), NATO ASI Series B, **250**, 339-339 Plenum Press, New York 1991.
2. A. Bongiorno, L. Colombo, F. Cargnoni, **C. Gatti**, M. Rosati, 'Coalescence and Organization of Self-Interstitial Clusters in Silicon', Proceedings of the 24th International Conference on the Physics of Semiconductors (ICPS-24), Jerusalem, 2-8 august 1998, World Scientific (1999).
3. L. Bertini, K. Billquist, M. Christensen, **C. Gatti**, L. Holmgren, B. Iversen, E. Mueller, M. Muhammed, G. Noriega, A. Palmqvist, D. Platzek, D.M. Rowe, A. Saramat, C. Stiewe, M. Toprak, S.G. Williams, Y. Zhang, 'Theoretical modeling of Te doped CoSb<sub>3</sub>', Proceedings of 22<sup>nd</sup> Int. Conf. on Thermoelectrics (2003), pages 85-88, IEEE Catalog Number 03TH8726, ISBN 0-7803-8301-X, ISSN 1094-2734.
4. L. Bertini, K. Billquist, M. Christensen, **C. Gatti**, L. Holmgren, B. Iversen, E. Mueller, M. Muhammed, G. Noriega, A. Palmqvist, D. Platzek, D.M. Rowe, A. Saramat, C. Stiewe, M. Toprak, S.G. Williams, Y. Zhang, 'Thermoelectric Properties of Nano-grained CoSb<sub>3</sub> Skutterudites Doped with Ni and Te', Proceedings of 22<sup>nd</sup> Int. Conf. on Thermoelectrics (2003), pages 48-51, IEEE Catalog Number 03TH8726, ISBN 0-7803-8301-X, ISSN 1094-2734.
5. L. Bertini, K. Billquist, M. Christensen, **C. Gatti**, L. Holmgren, B. Iversen, E. Mueller, M. Muhammed, G. Noriega, A. Palmqvist, D. Platzek, D.M. Rowe, A. Saramat, C. Stiewe, M. Toprak, S.G. Williams, Y. Zhang, 'Pitfalls in crystallographic analysis of doped skutterudite materials', Proceedings of 22<sup>nd</sup> Int. Conf. on Thermoelectrics (2003), pages 68-71, IEEE Catalog Number 03TH8726, ISBN 0-7803-8301-X, ISSN 1094-2734.
6. L. Bertini, K. Billquist, D. Bryan, M. Christensen, **C. Gatti**, L. Holmgren, B.B. Iversen, E. Mueller, M. Muhammed, G. Noriega, A.E.C. Palmqvist, D. Platzek, D.M. Rowe, A. Saramat, C. Stiewe, G. D. Stucky, G. Svensson, M. Toprak, S.G.K. Williams, Y. Zhang, 'Thermoelectric performance of large single crystal clathrate Ba<sub>8</sub>Ga<sub>16</sub>Ge<sub>30</sub>', Proceedings of 22<sup>nd</sup> Int. Conf. on Thermoelectrics (2003), pages 127-130, IEEE Catalog Number 03TH8726, ISBN 0-7803-8301-X, ISSN 1094-2734.
7. L. Bertini, K. Billquist, M. Christensen, **C. Gatti**, L. Holmgren, B. Iversen, E. Mueller, M. Muhammed, G. Noriega, A. Palmqvist, D. Platzek, D.M. Rowe, A. Saramat, C. Stiewe, M. Toprak, S.G. Williams, Y. Zhang, 'Grain Size Dependence of Transport Properties of Nano-engineered Thermoelectric CoSb<sub>3</sub>', Proceedings of 22<sup>nd</sup> Int. Conf. on Thermoelectrics (2003), pages 93-96, IEEE Catalog Number 03TH8726, ISBN 0-7803-8301-X, ISSN 1094-2734.
8. L. Bertini, K. Billquist, M. Christensen, **C. Gatti**, L. Holmgren, B. Iversen, E. Mueller, M. Muhammed, G. Noriega, A. Palmqvist, D. Platzek, D.M. Rowe, A. Saramat, C. Stiewe, M. Toprak, S.G.K. Williams, Y. Zhang, 'Standardisation in thermoelectric transport properties measurements - The Cardiff NEDO laboratories and DLR Cologne program', Proceedings of 22<sup>nd</sup> Int. Conf. on Thermoelectrics (2003), pages 532-536, IEEE Catalog Number 03TH8726, ISBN 0-7803-8301-X, ISSN 1094-2734.
9. L. Bertini, G. Borot, K. Billquist, M. Christensen, **C. Gatti**, L. Holmgren, B. Iversen, E. Mueller, M. Muhammed, G. Noriega, A. Palmqvist, D. Platzek, D.M. Rowe, A. Saramat, C. Stiewe, M. Toprak, S.G. Williams, Y. Zhang, 'Chemical Alloying and Characterization of Nanocrystalline Co<sub>1-x</sub>Ni<sub>x</sub>Sb<sub>3-y</sub>Te<sub>y</sub> Skutterudites', Proceedings of 22<sup>nd</sup> Int. Conf. on Thermoelectrics (2003), pages 117-120, IEEE Catalog Number 03TH8726, ISBN 0-7803-8301-X, ISSN 1094-2734.
10. S. Cenedese, L. Bertini, **C. Gatti** 'Ab-initio Modeling of Electronic Transport Properties in Filled (Ca, Sr, Ba) and Framework Substituted (Fe) Cobalt Antimonides', Proceedings ECT 2005, 3rd European Conference on Thermoelectrics, pages 53-55, September 1-2, 2005, Nancy, France.

11. S. Cenedese, L. Bertini, **C. Gatti** 'Ab-initio Modeling of Electronic Transport Properties in  $\text{Ca}_x\text{Co}_4\text{Sb}_{12}$ : the effect of the computational approach', Proceedings ECT 2005, 3rd European Conference on Thermoelectrics, pages 164-167, September 1-2, 2005, Nancy, France.

## List of IUCr conference papers published on Acta Cryst A

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1. **C. Gatti**, 'TOPOND : a program for the application of the quantum theory of atoms in molecules to periodic systems', Acta Cryst **A52**, C555 (1996).
2. **C. Gatti**, "Exploiting the theoretical electron and spin densities" Acta Cryst. **A56** (Supplement), s20 (2000).
3. G. K. H. Madsen, P. Blaha, K. Schwarz, J. Sofo and **C. Gatti**, 'LAPW Study of the Existence of Non Nuclear Maxima in the Electron Density', Acta Cryst. **A56** (Supplement), s187 (2000).
4. F. Cargnoni, **C. Gatti**, "Electron density topological analysis of silicon surfaces. The case of  $\text{Si}(100)(1\times1):\text{H}$  and  $\text{Si}(100)(2\times1):\text{H}$ " Acta Cryst. **A56** (Supplement), s402 (2000).
5. **C. Gatti**, L. Bertini, B.B. Iversen, N.P. Blake, "On the ionic Vs Neutral Nature of Metal Guests in the thermoelectric clathrate materials, Acta Cryst. **A58** (Supplement), C351 (2002).
6. **C. Gatti**, L. Bertini, F. Cargnoni, "Beyond  $\nabla^2\rho_b$  : chemical bond analysis using the local form of the source function", Acta Cryst. **A61**, C47-C48 (2005).
7. F. Cargnoni, L. Bertini, **C. Gatti**, "Structure, chemical bonding and thermoelectric performance of  $\text{Zn}_4\text{Sb}_3$ , Acta Cryst. **A61**, C349 (2005).
8. L. Bertini, S. Cenedese, **C. Gatti** "Ab-initio modelling of electronic transport properties: a structural informer", Acta Cryst. **A61**, C350 (2005).
9. **C. Gatti**, A.R Oganov, J. Chen, Y. Ma, " How and why elemental boron undergoes self charge transfer between 19 and 89 GPa " Acta Cryst. **A64** C70 (2008)
10. **C. Gatti**, Electron density topology and chemical bonding. The Quantum Theory of Atoms in Molecules and Crystals (Bader's theory), pages 91-115 ,International workshop on the refinement and analysis of the electron density obtained from high resolution X-ray diffraction, 28-30 October 2009, Marrakech, Maroc
11. **C. Gatti**, E. Monza, L. Lo Presti, G. Saleh " Revealing electron conjugation through an observable", Acta Cryst. **A67** C443-C444 (2011)
12. M.R.V. Jørgensen, S. Cenedese, H. F. Clausen, J. Overgaard, **C. Gatti**, Y.-S. Cheng, B.B. Iversen, " Charge density of a Zn containing coordination polymer", Acta Cryst. **A67** C447 (2011)
13. G. Saleh, **C. Gatti**, L. Lo Presti, J. Contreras-Garcia " Non-covalent interaction descriptor using experimental electron densities", Acta Cryst. **A67** C448-449 (2011)
14. S. Cenedese, **C. Gatti**, B.B. Iversen " Electronic structure and bonding interactions in  $\text{FeS}_2$  and  $\text{FeP}_2$ ", Acta Cryst. **A67** C449-C450 (2011)
15. **C. Gatti**, A.Orlando, L. Lo Presti, "Insights on spin-polarization via the spin density Source Function", Acta Cryst. **A70** C281 (2014)
16. A. Orlando, L. Loconte, E. Ortoleva, **C. Gatti**, L. Lo Presti, "Decoding conformational polymorphism in organic substances", Acta Cryst. **A70** C557 (2014)
17. G. Saleh, X. Dong, A. Oganov, **C. Gatti**, G. Qian, Q. Zhu, X. Zhou, H. Wang, "Stable Compound of Helium and Sodium at High Pressure ", Acta Cryst. **A70** C617 (2014)

18. **C. Gatti** "Solving chemistry puzzles in molecules and crystals through charge and spin density analyses", *Acta Cryst* A71, s5 (2015)
19. A. Orlando, **C. Gatti** and L. Lo Presti, "Non-Innocent role of ligands in some Ni organometallic complexes as viewed through the Spin Density Source Function", *Acta Cryst* (2015) A71, s416
20. **C. Gatti**, G. Macetti, L. Lo Presti, "Insights on spin density delocalization/polarization mechanisms through the source function", *Acta Cryst.* **A70**, C1434, (2017).

## Other publications

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1. M. Barzaghi, **C. Gatti**, 'Stabilita' relativa di strutture aromatiche e di Möbius', *Societa' Chimica Italiana, Sezione Lombardia, Riunione Scientifica* 3 dicembre 1986, *La Chimica e L'Industria* **69**, 98 (1987).
2. **C. Gatti**, 'Analisi della densita' elettronica ed effetto dell'impaccamento cristallino', pag. 271-336, in *Acquisizione, valutazione ed utilizzo di dati diffrattometrici e strutturali in Cristallografia*, Scuola 1994 dell'Associazione Italiana di Cristallografia, Perugia 3-7 ottobre 1994.
3. **C. Gatti**, 'Quantum Theory of Atoms in molecules and crystals. Application to the solid state', in *Hartree-Fock Theory of the Electronic Structure of Solids*, Network School of the Human Capital and Mobility Network on the 'Developments and Applications of the Hartree-Fock method in Materials Science', Turin (Italy), 17-27 September 1995.
4. **C. Gatti**, F. Cargnoni, 'Recent advances of the TOPOND program', **pagine 125-128**, *Atti III Convegno Nazionale di Informatica Chimica*, Napoli, 27 febbraio-1 marzo 1997.
5. **C. Gatti**, M. Cooper, 'Molecular and Crystal Properties from Charge and Spin Densities', *IUCr Newsletter*, **10**, issue 3, page 8-9 (2002).
6. G. K. H. Madsen, **C. Gatti**, B.B. Iversen, Lj. Damjanovic, G.D. Stucky, V.I. Srdanov "Erratum: F-Center in Sodium-Electro-Sodalite as a physical manifestation of a non-nuclear attractor in the electron density", *Phys. Rev. B* **61**, 2380-2380, (2000).
7. A. R. Oganov, V.L. Solozhenko, **C. Gatti**, O.O. Kurakevych, Yann Le Godec "Erratum: "The high-pressure phase of boron,  $\gamma$ -B28: disputes and conclusions of 5 years after discovery"" [*J. Superhard Materials*, **33**, no. 6, 2011], *J. Superhard Materials*, **34**, 74-74 (2012).
8. C. Gatti "Tavola periodica sotto pressione: una periodicit  diversa ed una chimica esotica", **Istituto Lombardo - Accademia di Scienze e Lettere - Incontri di Studio** [eISSN 2384-9878], ottobre 2019, <http://www.ilasl.org/index.php/Incontri/article/view/552>.

## Research Projects:

### International:

**1991-1993: Italian Head** of the CNR-CONICIT joined scientific cooperation agreement for the project *Relazioni tra misure di accoppiamento di quadrupolo elettrico nucleare e la topologia di densita' di carica teorica e/o sperimentale* (Relationships between the nuclear quadrupole coupling constants and the topology of the electron density obtained from ab-initio calculations or from X-ray diffraction data)

**1994-1997: Associated Contractor** of the EC Human Capital and Mobility Contract (CHRX-CT93-0155) "Developments and Applications of the Hartree-Fock Method to Materials Science". Dr. Gatti had the prime responsibility of implementing the Quantum Theory of Atoms in Molecules, due to R.F.W. Bader, to systems which are periodic in 0 up to three dimensions.

**2001-2003: Principal Contractor** of the project G5RD-CT2000-00292 on “Nano-Engineering of High Performance Thermoelectrics” within the EC 5<sup>th</sup> Framework Programme. Dr. Gatti had the prime responsibility to provide description of atomic interactions in molecular and crystalline thermoelectric materials, as an help to guide selection and optimization of these materials.

**2010-2020 : Carlo Gatti is one of the six international partners** of the Center for Materials Crystallography (CMC, <http://cmc.chem.au.dk/>), a new Centre of Excellence established January 1st, 2010, based on funding from The Danish National Research Foundation. The Center is headed by Prof. Bo Bummerstedt Iversen (Aarhus University, DK) and the six international partners are:

- Prof. Dr. Dietmar Stalke (Georg-August-Universität Göttingen, Germany)
- Prof. Mark Spackman (University of Western Australia, Australia)
- Dr. **Carlo Gatti** (Istituto di Scienze e Tecnologie Molecolari, Italy)
- Research Director Masaki Takata (SPring8 Synchrotron Facility, Japan)
- Exec. Director P. James Viccaro (University of Chicago Center for Advanced Radiation Sources, USA)
- Group Leader Bryan Chakoumakos (Neutron Scattering Division, Oak Ridge National Laboratory, USA)

The CMC is aimed at exploiting the revolutionising opportunities provided by new X-ray and neutron sources to tackle important challenges in materials science. These include:

- Unraveling the chemical origin of molecular self-assembly
- Understanding the mechanism behind thermoelectric materials capable of converting heat into electrical energy,
- Measuring structures of laser excited crystals
- Understanding the nucleation, growth and structure of the nanoparticles, which form the basis of emerging new energy technologies
- Quantifying how guest molecules interact with porous host materials used e.g. for gas storage or catalysis
- Obtaining an atomic scale insight into complex magnetic materials

The expertise and contribution of Dr Gatti within CMC concerns the ab-initio calculations of periodic systems, the development of new software implementing quantum topological approaches (such as Quantum Theory of Atoms in Molecules, QTAIM, Bader's theory) for the solid state and of new chemical bond descriptors, in particular the source function.

## National:

**1981: Appointed as Principal Investigator** (9 Months commitment) for the “*Studio di formazione e trasporto di prodotti di corrosione radioattivi in impianti LWR*” (Study of the formation and transport of radioactive corrosion products in LWR nuclear plants”, by **CNEN (presently ENEA)**, February 1981.

**1981: Appointed** (12 Months commitment) as a scientific counselor for the users of CILEA (Consorzio Interuniversitario Lombardo per la Elaborazione Automatica), charged and funded by **CILEA**, November 1981.

**1982 Appointed as Principal Investigator** (9 Months commitment) for the “*Studio sul meccanismo (formazione, trasporto, deposizione) della contaminazione radioattiva degli impianti BWR : miglioramento dei modelli e codici di calcolo esistenti, con particolare riferimento alla differenziazione morfologica e granulometrica del crud* (Study on the mechanism – formation, transport, deposition – of the radioactive contamination in the BWR nuclear plants: improvement of the existing models and computational codes, with a specific emphasis on the morphology and particle size of the crud” by **ANSALDO IMPIANTI**, divisione Meccanica Nucleare, April 1982.

**1989: Appointed as associated to the INFN** (sezione di Milano) for a research on the cold fusion to be held at the Laboratorio Nazionale del Gran Sasso, within a joined cooperation between the Laboratorio Nazionale del Gran Sasso (INFN), Università di Torino, Università di Milano, INFN sezione di Milano.

**1993-1994 Coordinator**, along with Prof. Carla Roetti, of the National Coordinated Project “*Verso lo sviluppo di software standardizzato per la modellistica di sistemi complessi* (Towards the development of a

*standardized software for the modelling of complex systems” (project funded by the Comitato Nazionale per la Scienza e le Tecnologie dell’Informazione, during the years 1993-96).*

**1995 : Appointed as Principal Investigator** of the project “Ideazione e sviluppo di SW per l’analisi topologica della densità elettronica in sistemi periodici (Development of a software for the topological analysis of the electron density in periodic systems)”, CNR, Comitato Nazionale Scienza e Tecnologie dell’Informazione.

**1998-2000 : Principal Investigator of the Operative Unit (Unità operativa)** of the project “Modelli e metodi per lo studio della struttura geometrica e di legame di difetti di silicio e di strati sottili di silicio clean o chemiadsorbiti (Models and methods for studying the geometrical and bonding structure of point and cluster defects in Silicon and in clean or chemisorbed Silicon slabs)”, **Progetto Finalizzato CNR Materiali Speciali per Tecnologie Avanzate II**, sottoprogetto 4, tematica 4.3 (Metodologie teoriche) (CNR project “Special Materials for Advanced Technologies II).

**2000: Head of an Operative Unit (Unità operativa)** within the project “Progettazione computazionale di cromofori NLO per il disegno mirato di sistemi fotorifrattivi ad alta efficienza (In silico design of NLO chromophores for highly efficient photorefractive systems”, Agenzia 2000, CNR.

**2006-2007 : CNR-ISTM Principal Investigator** of a joint project with Politecnico di Milano, Laboratorio di Micro/Nanoelettronica (Prof. Andrea Lacaita) on “*Non volatile semiconductor phase change memories*”, funded by CARIPLO, Fondi chiusi 2005, Project code : CARIPLO 2005-1245, Sector RICERCA SCIENTIFICA E TRASFERIMENTO TECNOLOGICO, Call 2005 on “Promuovere la valorizzazione della conoscenza attraverso il sostegno di progetti di ricerca applicata su tecnologie abilitanti”, Research in cooperation between Dip. di Elettronica e Informazione (DEI), Politecnico di Milano (P.I.: Prof. A. Lacaita) and CNR-ISTM ( P.I.: Dr. Carlo Gatti).