Curriculum Vitae: Dr. Bartolomeo Civalleri

Bartolomeo Civalleri was born in Cuneo (Italy) on September 6th, 1970.

He received his degree (Laurea, cum laude) in chemistry (1995) and his PhD in chemistry (1999) from the University of Torino (Italy) discussing a PhD thesis on "Hydrogen bond in molecular and crystalline systems: an ab initio study" under the supervision of Prof. P. Ugliengo.
After his PhD, he spent a short period working with Prof. N.M. Harrison at the CLRC Daresbury Laboratory (UK).
From 1999 to 2002 he worked as post-doc research assistant at the University of Torino, first, working with Prof. P. Ugliengo on "Ab initio modelling of zeolites" (1999-2000) and then, with Prof. C. Pisani and Prof. R. Dovesi, working on "Quantum-mechanical methods to study perfect and defective crystalline systems" (2001-2002).
Since 2002 he joined the Theoretical Chemistry Group (Department of Chemistry IFM) of the University of Torino as a faculty researcher.

Teaching activities
His teaching activities refer to computational chemistry and computational materials science for the master degree in chemistry and in materials science. Courses are on the fundamentals of ab initio computational chemistry of molecules and solids. He also gives lectures for short-course on Density Functional Theory.
He supervised several bachelor and master thesis and he is currently supervisor of two undergraduate students (master thesis) and a PhD student.
He also hosted a student (C. Argaez-Garcia) from Mexico within a project funded by the University of Torino.

Scientific activity (see list of publications for references)
His scientific activity is mainly devoted to ab initio modeling in solid state chemistry [1].

Since he joined the Theoretical Chemistry Group of the University of Torino in 2002, he has been involved in the development of the ab initio periodic code CRYSTAL (www.crystal.unito.it)[50] and is one of the co-authors of the last releases: CRYSTAL03, CRYSTAL06 and CRYSTAL09. He worked on developing parts of the code focusing on geometry optimization [65] and vibrational frequencies calculation [53] of periodic systems. He has collaborated with Prof. W. F. Perger (Michigan Tech University, USA) on the implementation of an automated tool for elastic constants calculation of crystalline systems [18]. In collaboration with C.M. Zicovich-Wilson, he has worked on the use of empirical corrections to include van der Waals interactions in DFT methods [27] and implementation of helical symmetry for one-dimensional systems [11]. Recently, he included in the code newly proposed GGA functionals for solids (e.g. PBEsol, SOGGA, ...) [5,16,30].

CRYSTAL is then used as a computational tool in the ab initio modeling of bulk and surface properties of various materials. His main scientific interests are: H-bond interactions in solids; adsorption phenomena in microporous materials as zeolites and metal-organic frameworks, bulk and surface properties of biomaterials and molecular crystals.

He has been working for many years on adsorption phenomena on silica and in microporous materials such as zeolites (see list of publications). During his PhD thesis, he proposed a simple periodic model of the surface of silica [75] that has been successfully applied to model the adsorption of ammonia [69], water [2] and biomolecules [43,25]. Recently, in collaboration with J. Torres, he explored the possible use of zeolites in both their acidic and cation-exchanged forms for di-hydrogen storage [29,38,39,46]. Interesting results were obtained when Mg^{2+} was adopted as adsorption site in good agreement with experimental findings [39].

Metal-organic frameworks has recently attracted a lot of interest for their use as adsorbants for hydrogen storage or carbon capture and storage but also for their potential role as semiconductors

for sensors, photocatalysis, electronics. Since 2005, he started a throughout investigation of MOFs: from MOF-5 [44] to recently synthesized Zirconium UiO-66 [87] and open metal CPO-27-M MOFs [9]. By working within European projects (MOFCAT and NANOMOF) in collaboration with Prof. S. Bordiga and C. Lamberti, a synergic combination of theory and experiment has allowed the full characterization of UiO-66, a highly stable and very promising MOF, and the study of the adsorption of CO, CO_2 and N_2 in Mg-MOF-74 in which the metal atom is exposed in the pore of the material [9].
He also recently showed the crucial role of dispersive interactions in the breathing of flexible MOFs such as MIL-53(Al) [3]. It has been clearly shown that the equilibrium between narrow pore and open pore phases is due to the competition between short-range and long-range interactions and entropic factors.
He is currently collaborating with Prof. J. Sauer on a detailed study of the energetics of adsorption of small molecules (CO and CO2) in CPO-27-M (M=Mg,Ni,Zn).
He is working on the prediction of the electronic properties of different IRMOFs by analyzing the role of the linkers in tuning the band gap of the material. Also, linear and nonlinear optical properties of MOFs and their elastic properties are under investigation because of their potential use in electronic devices as very low-k dielectrics.

Application of computational methods for understanding the structure and properties of molecular crystals [6,7,12,17,27,32,41,85,88] is another very interesting topic. Structural, cohesive, vibrational and dielectric (linear and nonlinear) properties of several molecular crystals have been investigated. In 2007, he clearly showed that commonly used DFT methods are not able to correctly describe the structure and cohesive energy of solid urea even if the crystalline structure is characterized by an extended network of hydrogen bonds [41]. The failure is due to the missing dispersive forces in the DFT functionals. Therefore, he worked to overcome this limit by adding an empirical dispersion correction to the B3LYP hybrid functional according to a proposal by S. Grimme. Very good results were obtained for a selected set of molecular crystals [27]. Recently this work has been extended including the comparison with periodic LMP2 results, by using the CRYSCOR program (www.cryscor.unito.it)[6,12]. In collaboration with Prof. A. Gavezzotti (University of Milan) he showed by comparing LM2, B3LYP-D* and PIXEL methods that affordable and reliable intermolecular interaction energies in organic materials can be obtained [88].
Recently, he has been working on the understanding of the role of crystal packing, and in particular of the hydrogen bonding, on linear and nonlinear optical properties of crystalline urea [17,85].

Within a national funded research project, he has collaborated with Prof. P. Ugliengo on the investigation of hydroxyapatite bulk and its (001) and (010) surfaces in relation to its role as a biomaterial. A fruitful collaboration with the group of Cristina Menziani at the University of Modena and Reggio Emilia (Italy) has allowed the development of a new force field apts to simulate the bulk and surfaces of hydroxyapatite. The Hench's bioglass has also been the subject of intense investigation in which classical molecular dynamics has been combined with B3LYP periodic calculation to predict structure and vibrational frequency of the bioglass.

He is also interested in following the developments of the Density Functional Theory. In particular, he is interested in DFT methods that provide a better description of weak interactions in solids. In this respect, the inclusion of a London-type empirical correction to DFT methods as proposed by S. Grimme has been applied to predict structure, energetics and vibrational properties of molecular crystals [27,15], layered materials [22], breathing of flexible metal-organic frameworks [3] and adsorption on surfaces [9,10] and in microporous materials [8] thus showing that the correct description of weak interactions is crucial for the ab initio modelling of solids.
He is now working on the implementation of both range-separated hybrid DFT methods, to be combined with post-HF techniques, and double-hybrids DFT methods.

Along this main stream, he has been involved in fruitful collaborations on:
1) *Vibrational analysis of polymers* (with Prof. G. Guerra, University of Salerno (Italy)). A combined computational and experimental study has allowed to fully characterize vibrational modes of polystyrene in two different conformations: trans-planar and s(2/1)2 helical [23,34,35]. An

assignment of the different modes was performed in terms of frequency, relative intensity, and direction of the transition-moment vector of the observed IR peaks as well as Raman vibrational frequencies. This was highly facilitated and validated by the experimental evaluation of the direction of the transition moment vector of most IR peaks, which was made possible for the first time by measurements on sPS films with different uniplanar orientations of the crystalline phase.
2) *Thermophysical properties of minerals* (with Prof. G. Ottonello, University of Genova (Italy)). By combining ab-initio calculation of vibrational frequencies and elastic constants with the Kieffer model to predict thermal expansion, heat capacity and thermodynamics properties of minerals (e.g. olivines and stishovite) [14,19,24,40]. This has been successfully applied to investigate and predict phase equilibria taking place at the Earth's mantle of interest for geophysical processes related to the so-called X-discontinuity in the mantle that, although sporadic, is found at 260-300 km depth in a range of mantle environments from seismic studies.

As a result of this broad research activity, he is co-author of more than 80 papers on peer-reviewed international journals (*h*-index=21, from ISI Web of Science).

Conference Organizer
He has organized the international schools "Ab-initio Modeling in Solid State Chemistry": MSSC2002, MSSC2003, and MSSC2006 held in Torino (Italy). He has been co-director of the most recent MSSC2007 and MSSC2009 schools (www.crystal.unito.it ⇒ events). He has also been invited as lecturer at MSSC-related international schools in Pau (F, 2003), Barcellona (E, 2004), Spokane (W, USA, 2006) and London (UK, 2008)
He has been co-chairman of the Microsymposia: Simulations of molecular crystals at the 26th European Crystallographic Meeting (Darmstadt (D), 29 August / 02 September 2010)

Other
He is member of the National Consortium of Materials Science and Technology (INSTM) which coordinates a network of 43 research units involving over 1800 affiliated scientists. He is also a member of the Nanostructured Interfaces and Surfaces (NIS) center of Excellence of the University of Torino.

He has contributed as reviewer for the following journals: Chemical Physics Letters, Journal of Chemical Physics, Journal of Physical Chemistry, Journal of Solid State Chemistry, Langmuir, Physica Status Solidi B, Physical Review B. He has also been a reviewer for NSF grants.

List of publications

Book chapters

1. Dovesi, R.; Civalleri, B.; Orlando, R.; Roetti, C.; Saunders, V. R., Ab initio quantum simulation in solid state chemistry. In *Reviews in Computational Chemistry, Vol 21*, ed.; Lipkowitz, KB; Raima, L; Cundari, TR Eds. **2005**; Vol. 21, 1-125.

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the alpha-beta-gamma polymorphs of Mg_2SiO_4: a computational study *Phys. Chem. Minerals* **2009**, 36 (2) 87-106
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and MP2 methods. *Journal of Physical Chemistry B* **1998,** 102, (13), 2373-2382.

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Articles in press or submitted

85. M. Ferrero, B. Civalleri, M. Rerat Polarizability and charge density distribution in crystalline urea. *J. Comp. Methods Sci. Eng.* (in press)
86. M. Prencipe, I. Scanavino, F. Nestola, M. Merlini, B. Civalleri, M. Bruno, R. Dovesi High pressure thermo-elastic properties of beryl ($Al_4Be_6Si_{12}O_{36}$) from ab initio calculations, and observations about the source of thermal expansion *Phys. Chem. Minerals* (in press)
87. L. Valenzano, B. Civalleri, S. Chavan, S. Bordiga, M. Nilsen, S. Jakobsen, K. P. Lillerud, C. Lamberti Disclosing the complex structure of UiO-66 MOF: a synergic combination of experiment and theory *Chem. Mater.* (submitted)
88. L. Maschio, B. Civalleri, P. Ugliengo, A. Gavezzotti Affordable and reliable intermolecular interaction energies in organic materials: mutual support between LMP2, dispersion-corrected DFT-D and PIXEL methods *Angew. Chem. Int. Ed.* (submitted)

Invited talks

1. *Density functional theory as applied to the study of hydrogen bonded systems*
   (Invited by Prof. G. Zerbi - Dipartimento di Chimica Industriale e Ingegneria Chimica, Politecnico di Milano, 1996)
2. *CRYSTAL03: a computational tool for solid state chemistry*
   (Invited by Prof. G. Ottonello - DIPTERIS, University of Genova, 14 May 2004)
3. *The problems of maintaining large codes: CRYSTAL*
   (Contribution to the round table on “New tools and technologies for computational chemistry”)
   (5th European Conference on Computational Chemistry, La Londe les Maures (F), 15-20 June 2004)
4. *Vibrations in crystalline urea: the role of the Hamiltonian*
   (Ab Initio Simulation of the Properties of Crystalline Surfaces and Interfaces: Progress and Prospects - 9th NIS Colloqium, Torino (I) 19-20 May 2005)
5. *Vibrational frequencies of crystalline compounds with the CRYSTAL code*
   (Contribution to the round table on “Molecular dynamics and multiscale methods”)
   (VII Convegno “Complex systems: structure, properties, reactivity and dynamics”, Alghero (Porto Conte Ricerche), 13-15 June 2005)
6. *Application of the CRYSTAL code to the study of hydrogen bonded molecular crystals*
   (IV European Charge Density Meeting, Brandenburg (D) 26-29 January 2006) [plenary]
7. *Ab initio quantum-mechanical investigation of molecular crystals*
   (* Microsymposia: Advanced methods for computer simulation of molecular crystals)
   (European Crystallographic Meeting, Leuven (B) 6-11 August 2006)
8. *Ab initio investigation of MOF-5*
   (MOFs: smart materials for catalysis and adsorption - NIS Colloqium, Torino (I) 15-16 February 2007)
9. *Recent developments of the CRYSTAL code and application to molecular crystals*

(Invited by Prof. S. Larsen - Department of Chemistry, University of Copenhagen, 18 December 2007)

10. *Vibrational properties of crystalline solids: ab-initio simulation and tools for their interpretation*
(Invited by Prof. C. Castiglioni - Dipartimento di Chimica, Politecnico di Milano, 26 June 2006, III Giornata "Metodi di caratterizzazione dei Materiali" del Dottorato in Ingegneria dei Materiali del Politecnico di Milano)
11. *Ab initio modelling of MOFs with the CRYSTAL code*
(Invited by Prof. G. Maurin - Institut Charles Gerhardt, University of Montpellier II, 12 June 2009)
12. *Ab initio modelling of the adsorption in microporous materials by means of the CRYSTAL code*
(Workshop on "Gas separation and gas storage using porous materials", CECAM, Lausanne (CH), 17-19 May 2010) [plenary]
13. *Effect of crystal packing on the static polarizability and first-hyperpolarizability of crystalline urea: An ab-initio computational study*
(* Microsymposia: Molecular interactions in crystal packing and molecular assemblies)
(26th European Crystallographic Meeting, Darmstadt (D) 29 August / 02 September 2010)

Invited Lectures (Schools)

1. MSSC2002 – Ab initio Modeling in Solid State Chemistry (Torino (I), 8-13 September 2002)
   - Introduction to the tutorial sessions – CRYSTAL input/output
   - Total energies, energy differences and geometry optimization
2. MSSC2003 – Ab initio Modeling in Solid State Chemistry (Torino (I), 7-12 September 2003)
   - Introduction to the tutorial sessions – CRYSTAL input/output
   - Total energies, energy differences and geometry optimization
3. Ecole d'automne de calcul ab initio dans les solides (Pau (F), 19-22 October 2003)
   - Overview of the CRYSTAL code. Basis sets: solutions and techniques
   - Total energies, energy differences and geometry optimization
4. Métodos ab initio para Sistemas Periódicos - Aplicaciones del programa CRYSTAL03- MASP2004 (Barcelona (E) 4-8 July 2004)
   - Hamiltonians (HF, DFT) and basis sets
5. MSSC2006 – Ab initio Modeling in Solid State Chemistry (Torino (I), 3-8 September 2006)
   - Introduction to the tutorial sessions – CRYSTAL input/output
   - Ab initio modeling of zeolites
6. ASCS2006 – Ab initio Simulation of Crystalline Systems (Spokane (USA), 17-22 September 2006)
   - Introduction to the tutorial sessions – CRYSTAL input/output
   - Total energies, energy differences and geometry optimization
   - Ab initio modeling of zeolites
7. MSSC2007 – Ab initio Modeling in Solid State Chemistry (Torino (I), 2-7 September 2007)
   - Introduction to the tutorial sessions – CRYSTAL input/output
8. MSSC2008 – Ab initio Modeling in Solid State Chemistry (London (I), 15-19 September 2008)
   - Introduction to the tutorial sessions – CRYSTAL input/output
   - Advanced options in geometry optimization and frequency calculation

Oral contributions (Congresses, Conferences, Workshops, ...) [co-authorship]

1. B. Civalleri, P. Ugliengo, E. Garrone
   Ab-initio quantum mechanical modelling of the silica hydroxyl groups by means of well designed cage cluster models
   (III International Symposium on Surface Heterogeneity in Adsorption and Catalysis, Torun (P), 9-15 August 1998)
2. P. Ugliengo, I. Roggero, B. Civalleri

Modelling the Brønsted acidity of H-Faujasite with the cluster approach and the ONIOM method
(International Workshop on Oxide-based Systems at the Crossroads of Chemistry, Villa Olmo, Como, 8-11 October 2000)

3. B. Civalleri, R. Orlando, C. Roetti, R. Dovesi
Recent developments of the ab initio periodic CRYSTAL code
(XXXI National Congress of Physical Chemistry, Padova, 19-23 June 2001)
4. B. Civalleri, P. Ugliengo
H-bonding at the silica surface modeled by ab initio calculations on clusters and periodic models
(Horizons in Hydrogen Bond Research XIV Conference-Workshop, Torino (I), 3-7 September 2001)
5. B. Civalleri
Periodic ab initio modeling of zeolites with CRYSTAL: the Chabazite framework as a case study
(XXI Congress of the Italian Chemical Society, Torino (I), 22-27 June 2003)
6. B. Civalleri
CRYSTAL03 as computational tool for solid state chemistry: from MgO to crambin
(GICC2003- V Edizione del Congresso del Gruppo Interdivisionale di Chimica Computazionale: dal Calcolo della Struttura Elettronica alla Bioinformatica - Siena (I), 18-19 December 2003)
7. B. Civalleri, J. Torres, C. Pisani
Ab initio modeling of hydrogen storage in microporous materials
(Seminario presso Regione Piemonte (Envy Park), 7 April 2005)
8. B. Civalleri, C. M. Zicovich-Wilson, L. Valenzano, P. Ugliengo
B3LYP augmented with an empirical dispersion term (B3LYP-D*) as applied to crystalline solids
(XXXVII National Congress of Physical Chemistry, Camogli (I), 24-29 February 2008)
9. B. Civalleri, C. M. Zicovich-Wilson, L. Valenzano, P. Ugliengo
B3LYP augmented with an empirical dispersion term (B3LYP-D*) as applied to molecular crystals
(5th European Charge Density Meeting, Gravedona (I), 6-11 June 2008)

Posters

1. B. Civalleri, P. Ugliengo, E. Garrone
Density functional study of hydrogen-bonded systems: application to gas-phase adducts and to catalytically relevant systems
(6th International Conference on Theoretical Aspects of Heterogeneous Catalysis, Tarragona (E), 2-7 giugno 1996)
2. P. Ugliengo, D. Viterbo, B. Civalleri, G. Chiari
MOLDRAW: a program for representing molecules and crystals on a personal computer
(III Convegno Nazionale di Informatica Chimica, Napoli, 27 febbraio - 1 marzo 1997)
3. S. Bordiga, F. Geobaldo, G. Spoto, D. Scarano, B. Civalleri, A. Zecchina
Evidence of repulsive interaction between Brønsted sites and hydrocarbon species with partial carbocationic character
(III International Symposium on Acid-Base Catalysis, Rolduc (NL), 20-24 Aprile 1997)
4. B. Civalleri, P. Ugliengo, E. Garrone
Spherohydridosilasesquioxanes as a model of silica and zeolite frameworks: an ab initio study
(II Convegno su “Ossidi semplici e misti come materiali innovativi”, Torino, 22-25 Giugno 1997)
5. R. Bianchi, G. Cicero, B. Civalleri, R. Orlando, P. Ugliengo, D. Viterbo
Studio teorico e sperimentale di solidi molecolari semplici
(XXVII Congresso Nazionale dell’Associazione Italiana di Cristallografia, Perugia, 12-14 Settembre 1997)

6. B. Civalleri, E. Garrone, P. Ugliengo, C. Pisani
   Ab initio quantum mechanical modelling of the silica hydroxyl groups by means of cage cluster models and extended periodic hydroxylated surfaces of edingtonite
   (7th International Conference on Theoretical Aspects of Heterogeneous Catalysis, Cambridge (UK), 25-28 agosto 1998)
7. P. Ugliengo, B. Civalleri, R. Dovesi, C.M. Zicovich-Wilson, V.R. Saunders
   Quantum mechanical calculations of the physico-chemical features of silica polymorphs
   (7th International Conference on Theoretical Aspects of Heterogeneous Catalysis, Cambridge (UK), 25-28 agosto 1998)
8. B. Civalleri, P. Ugliengo, C.M. Zicovich-Wilson, N.M. Harrison, R. Dovesi,
   Comparison between LCAO and plane wave ab-initio periodic calculations on H-Chabazite with variable Si/Al ratio
   (8th International Conference on Theoretical Aspects of Heterogeneous Catalysis, La Colle sur Loup (F), 31 maggio - 3 giugno 2000)
9. P. Ugliengo, I. Roggero, B. Civalleri
   Modelling the Brønsted acidity of H-Faujasite with the cluster approach and the ONIOM method
   (8th International Conference on Theoretical Aspects of Heterogeneous Catalysis, La Colle sur Loup (F), 31 maggio - 3 giugno 2000)
10. Roggero, B. Civalleri, P. Ugliengo
    Modeling physisorption with the ONIOM method: the case of NH3 at the isolated hydroxyl group of the silica surface
    (XXXI Congresso Nazionale di Chimica Fisica, Padova, 19-23 giugno 2001)
11. R. Orlando, B. Civalleri, R. Dovesi, C. Roetti, V.R. Saunders
    CRYSTAL a computational tool to characterize hydrogen bond in crystals
    (Horizons in Hydrogen Bond Research XIV Conference-Workshop, Torino (I), 3 - 7 settembre 2001)
12. B. Civalleri
    CRYSTAL: a computational tool to solid state chemistry
    (6th World Congress of Theoretically Oriented Chemists – WATOC2002, Lugano (CH), 4-9 agosto 2002)
13. C. Busco, G. Foddanu, B. Civalleri, P. Ugliengo
    Modeling Lewis acidity of a periodic (100) surface of Al-substituted Edingtonite
    (XXI Congresso della Società Chimica Italiana, Torino (I), 22-27 giugno 2003)
14. G. Croce, A. Arrais, E. Diana, M. Milanesio, B. Civalleri, D. Viterbo
    Validation of disordered crystal structures employing the periodic ab initio CRYSTAL code
    (XXI Congresso della Società Chimica Italiana, Torino (I), 22-27 giugno 2003)
15. S. Tosoni, B. Civalleri, P. Ugliengo
    Adsorption of water on crystalline silica surfaces: an ab-initio study using CRYSTAL03 periodic program
    (XVth International Conference on Horizons in Hydrogen Bond Research, Berlin (D), 16-21 settembre 2003)
16. S. Tosoni, B. Civalleri, P. Ugliengo
    Ab initio modeling of adsorption steps at silica surfaces
    (GICC2003- V Edizione del Congresso del Gruppo Interdivisionale di Chimica Computazionale: dal Calcolo della Struttura Elettronica alla Bioinformatica - Siena (I), 18-19 dicembre 2003)
17. B. Civalleri
    Computational Solid-State Chemistry with CRYSTAL: recent developments and applications
    (5th European Conference on Computational Chemistry, La Londe les Maures (F), 15-20 giugno 2004)
18. B. Civalleri
    Computational Solid-State Chemistry with CRYSTAL: recent developments and applications
    (LCC2004 - Local correlation methods: From molecules to crystals, Torino (I), 9-11 settembre 2004)
19. B. Civalleri, D. Viterbo, R. Bianchi, G. Croce, M. Milanesio, R. Orlando

Experimental and theoretical study of weak interactions in simple molecular solids
(XX Congress of International Union of Crystallography - IUCr2005, Firenze (I), 23-31 agosto 2005)

20. B. Civalleri
Ab initio HF and DFT investigation of crystalline urea
(11th International Conference on the Application of Density Functional Theory in Chemistry and Physics - DFT05, Geneva (CH), 11-15 settembre 2005)
21. B. Civalleri, C. Busco, M. Corno, P. Ugliengo
Ab-initio QM study on hydroxyapatite (001) and (100) surfaces
(V Convegno Nazionale sulla Scienza e Tecnologia dei Materiali, Geremeas-Maracalagonis, Cagliari (I), 26-29 settembre 2005)
22. J. Torres, B. Civalleri, R. Dovesi, C. Pisani
An ab-initio quantum mechanical study of the Al-substituted acidic chabazite as a candidate for hydrogen storage
(EHEC 2005- "2nd European Hydrogen Energy Conference", Zaragoza (Spain), 22-25 novembre, 2005)
23. J. Torres, B. Civalleri, P. Ugliengo, C. Pisani
An ab-initio study of the interaction of dihydrogen with microporous materials: chabazite zeolites and MOF-5
(11th International Conference on Theoretical Aspects of Catalysis, July 2006, Schmöckwitz, Germany)
24. M. Corno, C. Busco, B. Civalleri, A. Pedone e P. Ugliengo
Role of calcium hydroxyapatite in bioglasses: an ab-initio study
(European Conference Junior Euromat 2006, Losanna, 4-8 Settembre 2006)
25. J. Torres, B. Civalleri, P. Ugliengo, C. Pisani
An ab-initio study of the interaction of dihydrogen with microporous materials: alkali-exchanged chabazite zeolites
(MSSC2006 - Ab initio Modeling in Solid State Chemistry, 3-8 September 2006, Turin, Italy)
26. Pedone, M. Corno, B. Civalleri, G. Malavasi, U. Segre, P. Ugliengo, M.C. Menziani
A multi-scale approach to modelling of bioglasses
(XXII Congresso Nazionale della Società Chimica Italiana, Firenze, 10-15 settembre 2006)
27. M. Corno, A. Pedone, B. Civalleri, M. C. Menziani e P. Ugliengo
A computational multiscale approach to the modelling of 45S5 Bioglass®
(XXXVI Congresso Nazionale di Chimica Fisica, Gallipoli, 17-22 Giugno 2007)
28. J. Torres, B. Civalleri, P. Ugliengo, C. Pisani
Evaluation of the potential of proton- and metal-exchanged chabazites as media for molecular hydrogen storage: an ab initio study
(VII Congresso dell'Associazione Italiana Zeoliti, July 2007, Turin, Italy)
29. J. Torres, B. Civalleri, P. Ugliengo, C. Pisani
Evaluation of the potential of proton- and metal-exchanged chabazites as media for molecular hydrogen storage: an ab initio study
(MSSC2007 - Ab initio Modeling in Solid State Chemistry, 2-7 Settembre 2007, Turin, Italy)
30. Pedone, F. Musso, M. Corno, B. Civalleri, M. C. Menziani, U. Segre and P. Ugliengo
Periodic B3LYP study of hydroxylated crystalline silica surfaces as source for force field development.
(MSSC2007 - Ab initio Modeling in Solid State Chemistry, 2-7 Settembre 2007, Turin, Italy)
31. A.Ø. Madsen, B. Civalleri, F. Pascale, R. Dovesi, S. Larsen
Anisotropic displacement parameters for molecular crystals from periodic HF and DFT calculations
(5th European Charge Density Meeting, Gravedona (I), 6-11 giugno 2008)
32. L. Valenzano, F. Bonino, C. Lamberti, B. Civalleri
Ab-initio characterization of MOFs: M2(DOBDC) (M=Mg,Ni,Zn) and Zr-MOF (UiO-66,67,68) case studies
(VII Convegno Nazionale sulla Scienza e Tecnologia dei Materiali, Tirrenia, 9-12 giugno 2009)
33. L. Valenzano, F. Bonino, C. Lamberti, B. Civalleri

Ab-initio characterization of MOFs: M2(DOBDC) (M=Mg,Ni,Zn) and Zr-MOF (UiO-66,67,68) case studies
(MOFCAT Workshop "MOFs on the road to applications, Oslo (N), 17-19 giugno 2009)

34. M. De La Pierre, R. Demichelis, A.M. Ferrari, B. Civalleri, Ch. Manfredotti, C. Manfredotti
Differently oriented hydrogen terminated diamond surfaces: ab initio study of structure, energetics and vibrational spectra
(ESPA2010, Oviedo, (Spain) June 29-July 2, 2010)
35. L. Maschio, B. Civalleri, S. Casassa, R. Orlando, C. Pisani, R. Dovesi
CRYSTAL and CRYSCOR: two powerful tools for the ab-initio study of crystalline solids
(26th European Crystallographic Meeting, Darmstadt (D) 29 Agosto / 02 Settembre 2010)
36. M. De La Pierre, R. Demichelis, A.M. Ferrari, B. Civalleri, Ch. Manfredotti, C. Manfredotti
Differently oriented hydrogen terminated diamond surfaces: ab initio study of structure, energetics and vibrational spectra
(Diamond 2010, Budapest, (Hungary), September 5-9, 2010)
37. B. Civalleri, L. Valenzano, K. Sillar, J. Sauer
The adsorption of CO and CO2 on CPO-27-M (M = Mg, Ni, Zn) through quantum mechanical approaches
(2nd Int. Conference on MOFs and Open Framework Compounds, Marseille (F) September 5-8 2010)
38. B. Civalleri, L. Valenzano, S. Novarino, M. Ferrero, M. Rerat
Electronic properties of MOFs: an ab-initio investigation
(2nd Int. Conference on MOFs and Open Framework Compounds, Marseille (F) September 5-8 2010)
39. G.T. Palomino, S. Bordiga, S. Chavan, L. Valenzano, C. O. Arean, B. Civalleri
Thermodynamics of gas adsorption on Mg-MOF-74: combined theoretical and variable-temperature IR spectroscopic studies
(2nd Int. Conference on MOFs and Open Framework Compounds, Marseille (F) September 5-8 2010)

Other

1. V.R. Saunders, R. Dovesi, C. Roetti, R. Orlando, C. M. Zicovich-Wilson, N.M. Harrison, K. Doll, B. Civalleri, I. Bush, Ph. D'Arco, M. Llunell, *CRYSTAL03 User's Manual*, University of Torino, Torino, 2003
2. R. Dovesi, V.R. Saunders, C. Roetti, R. Orlando, C. M. Zicovich-Wilson, F. Pascale, B. Civalleri, K. Doll, N.M. Harrison, I. Bush, Ph. D'Arco, M. Llunell, *CRYSTAL06 User's Manual*, University of Torino, Torino, 2006
3. R. Dovesi, V.R. Saunders, C. Roetti, R. Orlando, C. M. Zicovich-Wilson, F. Pascale, B. Civalleri, K. Doll, N.M. Harrison, I. Bush, Ph. D'Arco, M. Llunell, *CRYSTAL09 User's Manual*, University of Torino, Torino, 2009
4. B. Civalleri and C. Roetti, editors, *CRYSTAL tutorial project - A tool for solid state chemistry and physics*, University of Torino, Torino, 2006