Lorenzo Maschio

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Associate professor at the Chemistry department of the **University of Torino** since 2017.

Author of 90+ published papers on international (ISI) journals and 3 book chapters. h-index: 27
10+ invited talks given at international conferences.

Winner of the 2018 **"Carla Roetti" prize** of the Theoretical and Computational Chemistry division of the SCI.

Main author of the **Cryscor** code (www.cryscor.unito.it) and of the most recent version of the **Crystal** code (www.crystal.unito.it).

My research activity always focused on the development of novel **methods and algorithms** for the **quantum-mechanical** simulation of **crystalline materials**, as well as the implementation of such methods in general purpose codes and its **application** to problems at the cutting edge of current research.

My current main research interests focus on:

- **Electron correlation methods** for periodic systems
- **Response** of solids to **electric and magnetic fields**
- Simulation of **transport properties** in solids
- Development and implementation of **dual basis set** techniques
- **Thermoelectric** materials
- Permanent **magnets**
- **Phosphorus**-based materials

Selected Publications

G. Sansone, A. J. Karttunen, D. Usvyat, M. Schutz, J. G. Brandenburg, **Lorenzo Maschio**
"On the Exfoliation and Anisotropic Thermal Expansion of Black Phosphorus"
ChemComm **54**(70), pp. 9793-9796

J. Linnera, G. Sansone, **Lorenzo Maschio**, A. J. Karttunen
"Thermoelectric Properties of p-Type Cu_2O, CuO, and NiO from Hybrid Density Functional Theory"
J. Phys. Chem. C, **122**(27), pp. 15180-15189

Lorenzo Maschio
"Direct inversion of the iterative subspace (DIIS) convergence accelerator for crystalline solids employing Gaussian basis sets."
Theoretical Chemistry Accounts, **137(4)**, 60 (2018)

D. Usvyat, **Lorenzo Maschio**, M. Schütz,

"Periodic and fragment models based on the local correlation approach",
Wiley Interdisciplinary Reviews: Computational Molecular Science, **e1357** (2018)

R. Dovesi, A. Erba, R. Orlando, C. M. Zicovich‐Wilson, B. Civalleri, **Lorenzo Maschio**, M. Rérat, S. Casassa, J. Baima, S. Salustro, B. Kirtman (2018).
"Quantum‐mechanical condensed matter simulations with CRYSTAL."
Wiley Interdisciplinary Reviews: Computational Molecular Science, **e1360** (2018).

G. Sansone, **Lorenzo Maschio** and A. J. Karttunen
"One-dimensional Phosphorus Nanostructures: from Nanorings to Nanohelices"
Chem. Eur. J. **23(63)**, 15884-15888 (2017)

G. Sansone, A. Ferretti and **Lorenzo Maschio**
"Ab initio electronic transport and thermoelectric properties of solids from full and range-separated hybrid functionals."
J. Chem. Phys. **147**, 114101 (2017)

D. Pullini, M. F. Sgroi, A. Mahmoud, N. Gauquelin, **Lorenzo Maschio**, A. M. Ferrari, R. Groenen, C. Damen, G. Rijnders, K. H. W. van den Bos, S. Van Aert, and J. Verbeeck
"One Step Toward a New Generation of C-MOS Compatible Oxide P–N Junctions: Structure of the LSMO/ZnO Interface Elucidated by an Experimental and Theoretical Synergic Work"
ACS Applied Materials & Interfaces **9 (24)**, 20974-20980 (2017) DOI: 10.1021/acsami.7b04089

C. Atzori, G. Shearer, **Lorenzo Maschio**, B. Civalleri, F. Bonino, C. Lamberti, S. Svelle, K.P. Lillerud, S. Bordiga
"The Effect of Benzoic Acid as Modulator in UiO-66 Structure: An Experimental and Computational Study"
J. Phys. Chem. C **121(17),** 9312–9324 (2017)

M. Schütz, **Lorenzo Maschio,** A. J. Karttunen, D. Usvyat
"The Exfoliation Energy of Black Phosphorus Revisited: A Coupled Cluster Benchmark"
J. Phys. Chem. Letters ***19****, 7699-7707* (2017)

A. J. Karttunen, D. Usvyat, M. Schütz and **Lorenzo Maschio**
"Dispersion Interactions in Silicon Allotropes"
Phys. Chem. Chem. Phys. **19(11)**, 7699-7707 (2017)

O. Masur, M. Schütz, **Lorenzo Maschio** and D. Usvyat,
"Fragment-based direct-local-ring-coupled-cluster doubles treatment embedded in the periodic Hartree-Fock solution"
J Chem. Theory Comput. ***12*** (10), 5145–5156 (2016)

Lorenzo Maschio, M. Rérat, B. Kirtman, R. Dovesi,
"Calculation of the dynamic first electronic hyperpolarizability β(−ωσ; ω1, ω2) of periodic systems. Theory, validation and application to multi-layer MoS2"
J. Chem. Phys. **143**, 244102 (2015), DOI:10.1063/1.4937770

D. Usvyat, **Lorenzo Maschio**, M. Schuetz,
"Periodic local MP2 method employing orbital specific virtuals"
J. Chem. Phys. **143**, 102805 (2015)

K. Sharkas, J. Toulouse, **Lorenzo Maschio**, B. Civalleri,
"Double-hybrid density-functional theory applied to molecular crystals"
J. Chem. Phys. **141**, 044104 (2014)

R. Dovesi, R. Orlando, A. Erba, C. M. Zicovich-Wilson, B. Civalleri, S. Casassa, **Lorenzo Maschio**, M. Ferrabone, M. De La Pierre, P. D'Arco, Y. Noël, M. Causà, M. Rérat, B. Kirtman

"CRYSTAL14: A program for the ab initio investigation of crystalline solids"
Int. J. Quantum Chemistry, **114**(19), 1287-1317 (2014), DOI: 10.1002/qua.24658

Lorenzo Maschio, Bernard Kirtman, Michel Rérat, Roberto Orlando, Roberto Dovesi.
"Ab initio analytical Raman intensities for periodic systems through a coupled perturbed Hartree-Fock/Kohn-Sham method in an atomic orbital basis. I. Theory."
J. Chem. Phys. **139**, 164101 (2013)

Lorenzo Maschio, Bernard Kirtman, Michel Rérat, Roberto Orlando, Roberto Dovesi.
"Ab initio analytical Raman intensities for periodic systems through a coupled perturbed Hartree-Fock/Kohn-Sham method in an atomic orbital basis. II. Validation and comparison with experiments."
J. Chem. Phys. **139**, 164102 (2013) – **Immagine di copertina** di questo numero della rivista

Cesare Pisani, Martin Schuetz, Silvia Casassa, Denis Usvyat, **Lorenzo Maschio**, Marco Lorenz, Alessandro Erba
"Cryscor: a program for the post-Hartree-Fock treatment of periodic systems"
Phys. Chem. Chem. Phys., **14**, 7615-7628 (2012)

Lorenzo Maschio, Bernard Kirtman, Roberto Orlando, Michel Rèrat
"Ab initio analytical infrared intensities for periodic systems through a coupled perturbed Hartree-Fock/Kohn-Sham method."
J. Chem. Phys. 137, 204113 (2012)

Marco Lorenz, **Lorenzo Maschio**, Martin Schuetz, Denis Usvyat
"Local ab initio methods for calculating optical bandgaps in periodic systems. II. Periodic density fitted local configuration interaction singles method for solids."
J. Chem. Phys. **137**, 204119 (2012)

Denis Usvyat, Bartolomeo Civalleri, **Lorenzo Maschio**, Roberto Dovesi, Cesare Pisani, Martin Schuetz
"Approaching the theoretical limit in periodic local MP2 calculations with atomic-orbital basis sets: The case of LiH."
J. Chem. Phys. **134**, 214105 (2011)

Lorenzo Maschio
"Local MP2 with Density Fitting for Periodic Systems: A Parallel Implementation."
J. Chem. Theory Comput. **7**, 2818-2830 (2011)

Lorenzo Maschio, Bartolomeo Civalleri, Piero Ugliengo, Angelo Gavezzotti
"Intermolecular Interaction Energies in Molecular Crystals: Comparison and Agreement of Localized Moller-Plesset 2, Dispersion-Corrected Density Functional, and Classical Empirical Two-Body Calculations."
J. Phys. Chem. A **115**, 11179-11186 (2011)

Martin Schuetz, Denis Usvyat, Marco Lorenz, Cesare Pisani, **Lorenzo Maschio**, Silvia Casassa, Migen Halo
"Density Fitting for correlated calculations in periodic systems"
In: Frederick R. Manby. Accurate Condensed-Phase Quantum Chemistry. p. 29-55, New York:CRC press - Taylor and Francis Group (2010)

Lorenzo Maschio, D. Usvyat, B. Civalleri
"Ab initio study of van der Waals and hydrogen-bonded molecular crystals with a periodic local-MP2 method."
CrystEngComm **12**, 2429-2435 (2010) – **invited paper**, special issue dedicated to new talents

Lorenzo Maschio, D. Usvyat, M. Schütz, B. Civalleri
"Periodic local-MP2 method applied to molecular crystals: Study of solid NH3 and CO2 using extended basis sets."

J. Chem. Phys. **132,** 134706 (2010)

Maschio Lorenzo, D. Usvyat
"Fitting of local densities in periodic systems."
Phys. Rev. B **78**, 073102 (2008)

C. Pisani, **Lorenzo Maschio**, S. Casassa, M. Halo, M. Schuetz, D. Usvyat
"Periodic Local MP2 Method for the Study of Electronic Correlation in Crystals: Theory and Preliminary Applications."
J. Comp. Chem. **29**, 2113-2124(2008)

Lorenzo Maschio, D. Usvyat, F. Manby, S. Casassa, C. Pisani, M. Schuetz
"Fast local-MP2 method with density-fitting for crystals. I. Theory and algorithms."
Phys. Rev. B. **76**, 075101 (2007)

D. Usvyat, **Lorenzo Maschio**, F. Manby, M. Schuetz, S. Casassa, C. Pisani
"Fast local-MP2 method with density-fitting for crystals. II. Test calculations and application to the carbon dioxide crystal."
Phys. Rev. B **76,** 075102 (2007)

C. Pisani, M. Busso, G. Capecchi, S. Casassa, R. Dovesi, **Lorenzo Maschio**, C. Zicovich-Wilson, M. Schuetz
"Local-MP2 electron correlation method for non conducting crystal."
J. Chem. Phys. **122**, 094113 (2005)