Lorenzo Maschio

Curriculum Vitae

- **PUBLICATIONS:**

  10**4** papers published on international (ISI) journals
  3 book chapters
  h-index: **31**
  ORCID ID: 0000-0002-4657-9439

- **AFFILIATIONS**

  Member of the Italian Chemical Society (SCI), membership card #**18108**

- **EDUCATION**

2003 – 2006	**Ph.D. in Materials Science and Technology**, University of Turin. Final dissertation (Quantum-mechanical ab initio computation of electronic correlation in crystalline solids) on December 4th, 2006. Supervisor prof.
1998 – 2003	**Master degree in Materials Science**, University of Turin. Title of the thesis: "Quantum-mechanical ab initio simulation of Oxygen-deficient centres in mixed SiO2-GeO2 glasses: two- and three-fold coordinated species" Supervisor prof. Cesare Pisani. Final mark: 110/110 cum laude

- **CURRENT POSITION**

2017 – **Associate Professor** in Physical Chemistry (CHIM02)
Department of Chemistry, University of Torino, Italy

- **PREVIOUS POSITIONS**

2010 – 2017 **Faculty Researcher** (Ricercatore Universitario) in Physical Chemistry (CHIM02)
Department of Chemistry, University of Torino, Italy

- **FELLOWSHIPS**

2006 – 2010 Postdoctoral grants, supervisor: prof. Cesare Pisani
Department of Chemistry, University of Torino, Italy

- **SUPERVISION OF GRADUATE STUDENTS AND POSTDOCTORAL FELLOWS**

2010 – 2020 Supervisor of 4 postdocs/ 3 PhD students/ 5 Master Students
Department of Chemistry, University of Torino, Italy

- **TEACHING ACTIVITIES**

2010 – Teaching courses of "**Physical Chemistry**", "**Environmental Chemodynamics**", "**Computers in Materials Science**" for Chemical and Materials sciences

- **GRANTS**

2020 PI of the UNITO unit of the MODALIS2 (MODelling of Advanced LI Storage Systems) project (coordinator: IFPEN, Lyon, France), funded 4.8 million euro within the H2020 programme of the European Commission, call LC-BAT-6-2019. UNITO budget: ~340 keuro

- **ORGANISATION OF SCIENTIFIC MEETINGS**

2017 Director of the MW-MSSC2017 international school– Minneapolis (U.S.A) 9-14 July 2017 ~50 participants. Co-organized with Laura Gagliardi http://www.crystal.unito.it/mw-mssc17/

2009 – 2020 Organizer of several schools in the MSSC series (see http://www.crystal.unito.it/events.php)

- **INSTITUTIONAL RESPONSIBILITIES**

2016 – Member of the scientific and management board of the **C3S inter-department centre** (Competence Centre for Scientific Calculus), University of Torino, Italy

2016 – Member of the scientific and management board of the **NIS inter-department centre** (Nanostructured Interfaces and Surfaces), University of Torino, Italy

2018 – Member of the Research Committee of the Chemistry Department of the University of Torino

- **MAIN SCIENTIFIC COLLABORATIONS**

Martin Schuetz, Denis Usvyat - Humboldt University, Berlin – Germany
Topic: electron correlation in solids with local methods

Bernard Kirtman - University of California at Santa Barbara – USA
Topic: Magnetic and electric field response in solids

Mauro Sgroi - FIAT Research Center - Torino, Italy
Topic: ab initio simulation of permanent magnets with low rare-earth content

Antti Karttunen – Aalto University, Finland
Topic: Simulation of thermoelectric materials, electron correlation in black phosphorus

Thomas Bondo Pedersen – University of Oslo - Norway
Topic: electron correlation in solids with local methods

- **SELECTED RECENT INVITED TALKS**

- **CECAM** workshop on non-covalent interactions, Lausanne (Switzerland), September 2021
"Local correlation in solids: the Cryscor code"
- **TMS2020**, **San Diego** (U.S.A.), 23-27 February 2020
"Ab-initio Study of TiMSn (M= Ni, Pt, Pd) Alloys using the CRYSTAL Ab-initio Package."
- **LCAMS2019**, **Regensburg** (Germania), 27-29 June 2019
"Ab-initio Study of TiMSn (M= Ni, Pt, Pd) Alloys using the CRYSTAL Ab-initio Package."
- **SIMPS2017** (Theoretical Chemistry for Periodic Systems: Systematically Improvable Electronic Structure Methods), **Tolouse** (Fr), 22-24 May 2017
"Recent developments in local correlation methods for periodic systems"
- **EMN** (Energy Materials Nanotechnology) Theory meeting, **Las Vegas** (USA), 10-14 October 2016
"The Tortoise and the Hare: Canonical and Local MP2 Implementations for Periodic Systems"
- **55th Sanibel Symposium** – St. Simon's Island GA – USA 14-20 February 2015 (**plenary talk**)
"Recent developments in local correlation methods for solids"

14/09/2021 Lorenzo Maschio

- **BRIEF DESCRIPTION OF SCIENTIFIC ACTIVITY**

My research activity is strongly focused on the **development** of new **methods and algorithms** for the quantum-mechanical simulation of **crystalline materials**, oriented towards the implementation in a general purpose, publicly distributed software. I am a main author of the **CRYSTAL17** release of the Crystal code (www.crystal.unito.it) and of the **CRYSCOR** program (www.cryscor.unito.it).

CRYSTAL is one of the most widely used codes for the *ab initio* (Hartree-Fock and DFT) study o **crystalline materials**, based on a **local** (Gaussian) **atom-centered basis set**. Developed since the '70s, as of today the code consists of more than 1 000 000 Fortran code lines and is used in hundreds of laboratories and industries worldwide.

Among all **my contributions** to the CRYSTAL code, the **most relevant** ones are:

- **Raman** and **Infrared** intensities through linear response (Coupled-perturbed - CPHF) approaches.
- Efficient **Convergence Accelerators** (DIIS) for iterative SCF and CPHF (first and second order) iterative procedures.
- Third-order response to dynamical electric fields (Pockels effect and **Second-Harmonic Generation**).
- **Transport properties** in solids (conductivity, Seebeck) through Boltzmann transport equations; **electron-phonon coupling**
- **Massively parallel** implementation of several algorithm, including electric field response.

CRYSCOR is an *ab initio* code for the treatment of **electron correlation** effects in crystalline solids, developed in the last 15 years through an intense collaboration between our group in Torino and the group of Martin Schütz in Germany. CRYSCOR, of which I am the **main developer**, is the first public software to implement accurate **local post-HF techniques** for solids. Its first public version was released in 2010, and as of today more than 100 licenses have been distributed worldwide.

The **major developments** I have personally coded in the CRYSCOR program during these years are:

- **Fast density-fitting electron evaluation** techniques for bielectronic integrals in crystalline systems, allowing for a gain up to four orders of magnitude in computing time.
- Efficient **parallel** (MPI) version of the code.
- **Local CIS** (Configuration Interaction Singles) for evaluating band gaps and excited states
- New techniques for an easier and more accurate description of the virtual manifold (**Orbital-Specific Virtuals**)
- Implementation of **"double hybrid"** functionals (density-scaled and range-separated).

Thanks to a **wide network of collaborations**, I am also involved in a number of apllicative studies of cutting-edge problems in the field of solid-state chemistry. This includes:

- evaluation of cohesive energies of **molecular crystals**
- relative stability of **polymorphs**
- correlation effects in nanostructured materials (**graphane, phosphorene**)
- simulation of **Infrared and Raman** spectra of materials (such as **Metal-Organic Frameworks**)
- magnetic solids and surfaces (LSMO, permanent magnets)
- **Thermoelectrics** (Half-Heusler alloys)
- Materials for **Li- Ion Batteries**