

Federico Brivio

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Summary

I hold a Research Fellowship at the Technion Institute of Technology (Haifa, Israel) in the group of prof. Dan Ritter and in Weizmann Institute (Rehovot, Israel) with in the group of prof. Leor Kronik. Here my research is focused on *ab-initio* modelling of electronic properties of semiconductors with a particular focus on modern theory of polarization.

I also have a position as visiting scientist at Charles University (Prague, Czechia). This is the continuation of my previous postdoctoral appointment in prof. Nachtigall group under the European project CUCAM. Here I personally supervise 2 PhD students and I coordinate the research work in close collaboration with experimentalists. In Prague I **designed and held a Master/PhD course** titled *Digital-age tools for research*. I was also co-responsible for two other classes: *Electronic Structure of Complex Molecular Systems and Biomolecules* and *Quantum Chemistry*. My research centres on pairing DFT calculations with molecular dynamics simulation to predict the catalytic properties of 2D materials and zeolites.

Previously I worked as postdoctoral researcher at the University of Cambridge (UK) under the supervision of FRS Sir. Prof. Anthony Cheetham and Dr. Paul Bristowe. In Cambridge I mainly worked in collabora-

tion with experimentalists to predict and rationalize experimental results such as: X-Ray/Neutron scattering diffraction, IR/Raman spectra and optical properties. I hold a PhD title in chemistry from the University of Bath. Here I was part of the **Marie Curie Project Destiny**; this has given me the opportunity to collaborate and observe different fields of research across Europe including industrial partners. Most of my research evolved around the study of hybrid perovskites for photovoltaic applications. I used computational techniques and theories to tackle different aspects of the physics of these materials and invest(ed) my energies in the cause of **environmental sustainability**.

I have engaged with schools and public audiences through various activities such as ScienceSlam in Prague, BathTapsIntoScience in Bath, and the **Three Minute Thesis competition**. My actual position is also the natural continuation of my Master's and Bachelor degree in Materials Science in Milano Bicocca University. This offered me a multi-disciplinary curriculum in both Chemistry and Physics of the Solid State and I think my experiences reflect my lifelong inclination towards science. As a computational scientist I advocate for open science and open software principles.

Position and Education

Technion – Israel Institute of Technology

Postdoctoral Fellow

- Member of prof. **Leor Kronik** and prof. **Dan Ritter** groups
- Calculations of Polarization constant in GaN using the modern theory of polarization (Berry Phase)

HAIFA, ISRAEL

Jan 2021 – present

Charles University

Visiting Scientist

- I continue the supervision of PhD students and the research project on *ab-initio* NMR simulations.

PRAGUE, CZECHIA

Jan 2021 – present

Charles University

PostDoctoral research assistant

- Supervisor: prof. Petr Nachtigall
- I worked in Prague with the *International Mobility of Researchers* part of the European investment funding for development of education for 18 months. After this I became part of the *Charles University Centre of Advanced Materials* (CUCAM). Besides my teaching and research duties I strongly collaborate with experimental research groups of Prof. Jiri Cejka and Prof. Russel Morris,FRS (St. Andrews, UK).
- Lecturer of *Digital-age tools for research* and co-lecturer of Master/PhD classes

PRAHA, CZECHIA

May 2018 – Dec 2021

University of Cambridge

PostDoctoral research assistant

- Supervisor: Prof. Sir Anthony Cheetham and Dr. Paul Bristowe
- As a PostDoctoral researcher I focused on DFT calculation in strong collaboration with the experimental group of Prof. Cheetham
 - Supervision of first year students in *Material Science* classes
 - Clare college Supervisor
 - Prediction of crystal structure to support X-ray/Neutron scattering data
 - Thermodynamic simulations for extreme condition of synthesis

CAMBRIDGE, UK

Oct 2016 – Oct 2017

University of Bath

PhD student

BATH, UK

Nov 2012 – Jun 2016

- Supervisor: Prof. Aron Walsh and Prof. Alison Walker
- Thesis title: *Ab-Initio atomistic modelling of hybrid perovskites for solar cells.*
- In March 2013, after a few months at Bath University in Walsh's group, I joined the **DESTINY Marie Curie Initial Training Network**. Being part of this European platform permitted me to experience the reality of large collaboration networks and their management mechanisms.
 - I investigated three main aspect of hybrid perovskites: electronic structures, vibrational, and thermodynamic properties
 - DFT calculations: VASP, FHI-AIMS, Gaussian, Crystal and MOLCAS
 - Supervision of master students. Tutoring of students in computational chemistry and programming labs
 - External collaboration Dyesol, Roma Tor Vergata University - Chose
 - Public engagement: Bath taps into science, interactive laboratory, Three Minute Thesis (vimeo.com/155831465), ...

Università degli Studi di Milano-Bicocca

Masters and Bachelor

MILANO, ITALY

2006-2011

- Laurea Magistrale in Scienza dei materiali - Master degree in Materials Science: 2009 – 2011
 - Supervisors: Prof. **Gianfranco Pacchioni** and Dr. **Cristiana Di Valentin** - Thesis title: *Electronic structure of organic systems for electrochromic applications*
- Laurea Triennale in Scienza dei materiali - Bachelor degree in Materials Science: 2006 – 2009
 - Supervisor: Prof. **Michele Catti** - Thesis title: *Modelling of structural and transport properties of Lithium and Iron oxides*
- Institut de Química Teòrica i Computacional (Barcelona, ES): April 2011 – August 2011
 - Study of multiconfiguration wavefunctions with the software MOLCAS in the group of prof. **Francesc Illas** and Dr. **Carmen Sousa**

Experience

- Member of projects **review-panel** for the *Deutsche Forschungsgemeinschaft (DFG)* on hybrid perovskites
- Peer-review of several high-impact international journals for several editors
- **Dyesol** (Manchester, UK) External collaborator: 2012-2016
 - **Dyesol** is a worldwide leader in third generation photovoltaic. During my stay I helped to rationalize the choice of materials for the development of new contacts for hybrid perovskites solar cells.
- **Università degli Studi di Roma Tor Vergata** (Roma, IT) - Visiting student: April 2014-May 2014
 - Collaboration on the development of TiberCad code
- **Scuola Media Statale A. Volta** (Robbiate, IT) - Teacher of Natural Sciences and Maths, including didactic laboratories (75 pupils aged 11-14 years old).

Award and conferences

- Recipient as main investigator for PRACE-DECI16 and PRACE-DECI17 awards to grant access to the European supercomputer network.

Being part of an European Initial Training Network (ITN) gave me the opportunity from an early stage to present my work in different universities, and to be involved in the Management meetings of the project. I interacted directly with the PIs of the project and with the European Institutions delegates. I had given oral presentations in European universities. A partial list of the most significant ones:

- **Best Talk:** 2st International Conference on Perovskite Solar Cells and Optoelectronics (PSCO), Genova IT, 26-28 September 2018
- **Invited speaker:** Workshop on low dimensional materials, Liblice Castle CZ, 8–11 September 2020
- **Speaker** Conference: 14th International Conference on Materials Chemistry (MC14), Birmingham UK, 8-11 July 2019
- **Speaker** Conference: 2016 MRS fall Meeting and Exhibit, Boston, USA. 27 November - 2 December 2016

- **Speaker** Conference: 12th International Conference on Materials Chemistry (MC12), University of York, UK 20-23 July 2015
 - **Speaker** ITN Meeting: Midterm review meeting, Bruxelles BE. 21 October 2014
 - **Workshop**: Photoelectrochemistry Meeting, University of Bath, Bath UK, 04-06 September 2013
 - **Invited speaker Summer School**: Collaborative Computational Project for condensed phase physics (CCP5) Summer School, Manchester University, UK 21-30 July 2013
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Skills

Languages: Italian (mother tongue), English (professionally fluent - C1), and Spanish (basic)

Computer skill: I am proficient user of **VASP**. Nonetheless I performed different calculations and post-processing with FHI-AIMS, Crystal, Gaussian, PhonoPy, TiberCAD, Atomic Simulation Environment (ASE), ...

I usually program small codes in Fortran77-90 and I have basic knowledge of Python. My operating system of election is Linux. I generally use Bash, gnuplot, \LaTeX (including this document) and Beamer.