Federico Brivio

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Summary

I submitted my PhD thesis and my graduation is expected the 15^{th} of July. I am part of the **Marie Curie Project Destiny**; this has given me the opportunity to collaborate and observe different fields of research across Europe. I have also been an active part of the project management. My research focuses mostly on **hybrid perovskites**. These materials are employed as light harvesters in photovoltaic devices. Interest in hybrid perovskite exploded during my PhD and allowed me to engage in a highly competitive and dynamic subject. To study the processes behind such novel materials required me to develop thinking at the forefront of science and this aspect in particular gave me an additional thrill. I used varied computational techniques and theories to tackle different aspects of the physics of these materials. This led me to publish papers and present my work to at a number of international conferences. I have engaged with schools and public audiences through various activities. Recently I took part in the Three Minute Thesis competition where I explained the aim of my research in under 3 minutes. Before starting the PhD, I also spent a few months as a teacher in junior school. I obtained **Bachelor** and **Master's degrees** in **Materials Science** from Milano Bicocca University. This offered me a multidisciplinary curriculum in both *Chemistry* and *Physics of the Solid State*. During my thesis I specialised in computational simulations of crystalline and molecular systems. In my final year I also spent six months at the *Institute of Theoretical and Computational Chemistry* in Barcelona with the **Erasmus** project. This particular experience introduced me to an international research environment. My experiences reflect a lifelong inclination towards science. Before university I attended the *Liceo Scientifico* within the *National Informatics Plan* (a curriculum with more Maths and Informatics hours). This was my first experience of programming (PASCAL) and I joined the student informatics committee where I contributed to creating and managing the school website. In this period I also started to use Linux systems and I became acquainted with the free software philosophy. During my junior school education I followed optional classes such as computer science and natural science laboratories. I have had the opportunity to use computers since the MS-DOS era and have been engaged ever since.

Education

- University of Bath — Bath, UK
  PhD: *Ab-Initio* atomistic modelling of hybrid perovskites for solar cells. *Nov 2012 – Exp. June 2016*
  Supervisors: Prof. **Aron Walsh** and Prof. **Alison Walker**
  In March 2013, after a few months at Bath University in the group of Prof. Aron Walsh, 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 structure** using different levels of theory to describe the anomalous effects of hybrid perovskites (e.g. **Rashba** effect).
    - **Vibrational properties** (using Phonopy) to obtain simulated IR/Raman Spectra and phonon dispersion. This has been performed using different levels of theory such as the **finite displacement method**, **density functional perturbation theory** and **quasi-harmonic approximation**.
    - Thermodynamic properties (i.e. phase diagram) of mixed composition perovskites using the **generalized quasi-chemical approximation**.
  - DFT calculations:**VASP**, FHI-AIMS, Gaussian, Crystal and MOLCAS.
  - Using high performance computing platforms with **task-farming**.
  - Scripting:**Bash**, **Fortran**, **gnuplot** and **python**.
  - Writing and publishing my results. My publication record is available here: Federico Brivio on Google Scholar
  - **Peer reviewer**.
  - Supervision of master students.
  - Tutoring of students in computational chemistry and programming labs.
  - External collaboration Dyesol (commercial), Roma Tor Vergata University (academic).
  - Public engagement:Bath taps into science, interactive laboratory, Three Minute Thesis (vimeo.com/155831465).

• Università degli Studi di Milano-Bicocca — Milano, Italy

Laurea Magistrale in Scienza dei materiali - Master degree in Materials Science *2009 – 2011*

Supervisors: Prof. **Gianfranco Pacchioni** and Dr. **Cristiana Di Valentin**.
Thesis title: "Struttura elettronica di sistemi organici di interesse per applicazioni elettrocromiche - 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: "Modellizzazione di proprietà strutturali e di trasporto di ossidi di ferro e litio - Modelization of structural properties of lithium iron oxides".

Institut de Química Teòrica i Computacional *Barcelona, Spain*

Erasmus Student *April 2011 - August 2011*

- Collaboration during my master with the supervision of Dr. **Carmen Sousa**.
- Performed beyond DFT calculation (CASPT2 with MOLCAS).

Experience

• Università degli Studi di Roma Tor Vergata — Roma, Italy

Visiting student *April 2014-May 2014*

- Interaction with collaborating group.
- **Continuum calculations** with the software TiberCAD applied to perovskite materials.

• Dyesol — Manchester, UK

External collaborator

Dyesol is a worldwide leader in third generation photovoltaic. During my stay I helped to rationalise the choice of materials for the development of new contacts for hybrid perovskites solar cells.

- Collaboration within a **commercial environment**.
- Rationalising/directing the choice of contact materials.

• Scuola Media Statale A. Volta — Robbiate, Italy

Teacher *April 2012 - June 2012*

- 75 students aged between 11 and 14 years old.
- Teaching of Natural Sciences and Maths, including didactic laboratories.

Conferences and courses

Being part of an European Initial Training Network (ITN) gave me the opportunity not only to present my work in different universities, but also 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:

- Conference: **12^{th} International Conference on Materials Chemistry (MC12)**, University of York, United Kingdom. *20-23 July 2015*
- ITN Meeting: **Annual meeting year 2**, Oxford, Belgium. *19-21 January 2015*
- ITN Meeting: **Midterm review meeting**, Brusseles, Belgium. *21 October 2014*
- ITN Meeting: **Midyear meeting year 2**, Castellon, Spain. *09-13 June 2014*
- ITN Meeting: **Annual meeting year 1** Athens, Greece. *07-11 January 2014*
- Workshop: **MTG-MICE 3**, Bath, United Kingdom. *04-06 September 2013*
- Workshop: **Photoelectrochemistry Meeting**, University of Bath, Bath, United Kingdom. *04-06 September 2013*
- Summer School: **Collaborative Computational Project for condensed phase physics (CCP5) Summer School** (Invited speaker), Manchester University, United Kingdom. *21-30 July 2013*
- ITN Meeting: **Midyear meeting Year 1**, Ventotene, Latina, Italy. *03-07 June 2013*
- ITN Meeting: **Kickoff Meeting**, University of Bath, Bath, United Kingdom. *29-30 January 2013*

I also attended the following conferences:

- Conference: **The Frontiers of Materials Modeling - TYC 10th Anniversary Symposium**, London, United Kindom. (Poster) *17-19 February 2016.*
- Conference: **Next Generation Materials for Solar Photovoltaics**, London, United Kindom. (Poster) *25 January 2016.*
- Conference: **1st International Conference on Perovskite Solar Cells and Optoelectronics (PSCO)**, Lausanne, Switzerland. (Poster) *27-29 September 2015.*
- Conference: **Psi-k 2015**, San Sebastian, Spain. (Attendance) *06-10 September 2015*
- Workshop: **CECAM: Perovskite solar cells: the quest for a theoretical description**, Lausanne, Switzerland. (Attendance) *25-28 August 2015*
- Conference: **The 7th International Conference on Hybrid and Organic Photovoltaics (HOPV)**,Rome, Italy. (Poster) *10-13 May 2015*
- Summer school: **Impedance Spectroscopy School**, Castellon, Spain. (Attendance) *9-13 June 2014*
- Course: **LMF/QSGW Hands-On Course**, STFC Daresbury Laboratory, Warrington, United Kingdom. (Attendance) *17-19 March 2014*
- Workshop: **Frontiers in Modelling Optical Excitations of Materials Workshop TYC**, Chicheley, United Kingdom. (Attendance) *04-06 September 2013.*
- Conference: **11^{t}h International Conference on Materials Chemistry (MC11)**, University of Warwick, United Kingdom. (Poster) *08-11 July 2013*
- Conference: **The 5th International Conference on Hybrid and Organic Photovoltaics (HOPV)**,Seville, Spain. (Poster) *05-08 May 2013*
- Course: **Fortran 95**, University of Warwick, UK. (Attendance) *10-12 December 2012*

Skills

Natural languages: Italian *(mother tongue)*, English*(fluent)*, and Spanish *(basic)*.

Computer skill: During my PhD I mostly used **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, LaTeXand **Beamer**.

Interests

Non-exhaustive and in alphabetical order: Art, basketball, cinema, cooking, computer science, economy, free software, half-marathons runner, music, photography, public engagement, technology, travel.

Publications

[1] **Brivio, Federico**, Alison B Walker, and Aron Walsh. "Structural and electronic properties of hybrid perovskites for high-efficiency thin-film photovoltaics from first-principles". In: *APL Materials* 1.4, 042111 (2013).

[2] Jarvist M Frost, Keith T Butler, **Brivio, Federico**, Christopher H Hendon, Mark Van Schilfgaarde, and Aron Walsh. "Atomistic origins of high-performance in hybrid halide perovskite solar cells". In: *Nano letters* 14.5 (2014), pp. 2584–2590.

[3] **Brivio, Federico**, Keith T Butler, Aron Walsh, and Mark Van Schilfgaarde. "Relativistic quasiparticle self-consistent electronic structure of hybrid halide perovskite photovoltaic absorbers". In: *Physical Review B* 89.15 (2014), p. 155204.

[4] **Brivio, Federico**, Jarvist M Frost, Jonathan M Skelton, Adam J Jackson, Oliver J Weber, Mark T Weller, Alejandro R Goñi, Aurélien MA Leguy, Piers RF Barnes, and Aron Walsh. "Lattice dynamics and vibrational spectra of the orthorhombic, tetragonal, and cubic phases of methylammonium lead iodide". In: *Physical Review B* 92.14 (2015), p. 144308.

[5] Ralf G Niemann, Athanassios G Kontos, Dimitrios Palles, Efstratios I Kamitsos, Andreas Kaltzoglou, **Brivio, Federico**, Polycarpos Falaras, and Petra J Cameron. "Halogen Effects on Ordering and Bonding of CH3NH3+ in CH3NH3PbX3 (X= Cl, Br, I) Hybrid Perovskites: A vibrational spectroscopic study". In: *The Journal of Physical Chemistry C* (2016).

[6] **Brivio, Federico**, Clovis Caetano, and Aron Walsh. "Thermodynamic Origin of Photoinstability in the CH3NH3Pb (I1–x Br x) 3 Hybrid Halide Perovskite Alloy". In: *The journal of physical chemistry letters* 7 (2016), pp. 1083–1087.

References

Prof. Aron Walsh

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Note	Prof. Aron Walsh will be moving to Imperial College London in September 2016.

Prof. Alison Walker

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