Curriculum Vitae Bernardino Tirri

Tel: +39 345 32 32 459
e-mail: bernardino.tirri@chimieparistech.psl.eu
Date of birth: 21/12/1989
Skype: bernardino.tirri
Nationality: Italian

11, Rue Pierre et Marie Curie
Équipe Chimie Théorique et Modélisation iCLeHS, FRE 2027
ChimieParisTech 75005 Paris, France

Education and training

Feb 2018 – Current
PhD in Computational Chemistry

Dec 2015 – Jun 2018
Master degree in Chemical Science

(Final Grade: 110/110)

Università degli Studi di Napoli " Federico II" - Napoli (Italy)

Bernardino background research revolves around the electrochemical properties of cutting edge materials for energy conversion/storage devices via state-of-the-art computational methods. Since October 2018 Bernardino moves in Paris to work within Theoretical Chemistry and Modelling group (CTM) at the *Ecole Nationale Superieure de Chimie de Paris* (*ENSCP*), in order to develop new tools able to predict pertinent physico-chemical properties of the dyes developed by PILI company. Furthermore, he is an elected member of management board within the *ENSCP*. Since 2015 he is a member of the Italian Chemistry Society.

Research Experience

PhD in Computational Chemistry

Title: *"Determination of a computational protocol for the prediction of UV-vis spectra of molecules in solution"*

Project abstract:
Industrial dyes used in the textile industry are mainly derived from petroleum showing therefore a not negligible environmental impact all along their production cycle. Investigations have been therefore undertaken on colorants derived from clean bio-resources having a minimal ecological negative impact. In particular, a promising way is represented by use of microorganism in dye production. These bio-sourced molecules are specially designed to mimic the existing industrial dyes, which ensures their good performance. However, the optical properties of such a dyes cannot be easily a priori predicted without using accurate and robust computation protocols.

The objective of this PhD project is to develop a predictive computational tool enabling to access key features of the UV-Visible spectrum of the categories of molecules of interest for the PILI company. The expertise of the CTM team in modelling of excited state of molecules in solution and in more complex environments will allow to setup during the PhD thesis an approach rooted on first principle methods, able to predict with sufficient accuracy several physico-chemical properties of the chromophore of interest including, in particular, the maximum absorption wavelength (λ_{max}), the molar extinction coefficient (ε) as well as the band shape profile of the UV-Vis absorption spectra. With this tool in hand, tested and validated on a relevant set of know compounds, a low cost fully in-silico design of new chromophore candidates will be then developed.
Supervisor: Carlo Adamo
Theoretical Chemistry and Modelling, Chimie ParisTech - Paris (France)

CNRS Computational Engineer

TD-DFT calculations on Organic Dyes.
Supervisor: Carlo Adamo
Theoretical Chemistry and Modelling, Chimie ParisTech - Paris (France)

Master Thesis

Thesis Title: *"Ab Initio Study of Structure-Property Relationships in Disordered $LiCo_{1/3}Fe_{1/3}Mn_{1/3}PO_4$ Olivine for Li-ion Batteries."*

Supervisors: **Ana Belén Muñoz-García**
Co-Supervisors: **Michele Pavone**
Sergio Brutti
Università degli Studi di Napoli "Federico II" - Napoli (Italy)

Bachelor Thesis

Thesis Title: *"Mechanism of Oxygen Evolution Reaction on Fe-based perovskite oxides: towards effective electrocatalysis of water splitting."*

Supervisors: **Ana Belén Muñoz-García**
Co-Supervisor: **Michele Pavone**
Università degli Studi di Napoli "Federico II" - Napoli (Italy)

Scientific Publications

Conferences

XV Sigma-Aldrich Young Chemists Symposium (Saycs 2015). Rimini, 27-29/10/ 2015. Title: *Mechanism of Oxygen Evolution Reaction on Fe-based perovskite oxides: towards effective electrocatalysis of water splitting*.

XLIV Congresso Nazionale di Chimica Fisica. Napoli, 20-23/09/2016. Title: *First-principles study of oxygen evolution and reduction reactions on the stoichiometric and defective LaFeO3 (001) surface*.

Workshop ERC " Development of a Research Environment for Advanced Modelling of Soft Matter. Capri (Na), 20-22/04/2017. Title: *Oxygen reactivity at the stochiometric and defective LaFeO3 (001) surface*.

XXVI Congresso Nazionale della Società Chimica Italiana. Paestum (Sa), 10-14/09/2017. Title: *First- Principles Study of the Lanthanum Ferrite Surface Chemistry Toward Oxygen Evolution/Reduction Reaction*.

Manuscript in preparation

Title: *Unveiling structural, electronic and defect properties of LiCo(1/3)Fe(1/3)Mn(1/3)PO4, a high performance cathode for Li-ion batteries*. Authors: Ana Belen Muñoz Garcia, Bernardino Tirri, Isaac Capone, Michele Pavone*, Sergio Brutti*.

Technical Skills and Competences

- **DFT packages**: *Vienna ab initio simulation Package, Gaussian;*
- **Visualization and Data Analysis**: *Vesta, Gaussview, VMD, xmgraces;*
- **Knowledge in programming languages**: Perl, *Python, AWK, Bash/shell scripting;*
- **Knowledge stochastic code:** *ATAT; LAMMPS;*
- **Graphic design application:** *Photoshop;*
- **Knowledge of Microsoft Office Package;**
- **Operative system:** Linux, macOs, Windows;

Languages:

Mother tongue: Italian

Fluent in English

Beginner in French

References

Carlo Adamo *carlo.adamo@chimie-paristech.fr*
Michele Pavone *michele.pavone@unina.it*
Ana Belén Muñoz-García *anabelen.munozgarcia@unina.it*