

Mariarosaria Tuccillo

Curriculum vitae

Current Position

November 2020 – Now **PhD Student** in Chemical Processes for Industry and the Environment – University of Rome “La Sapienza”.

Topic: "Novel positive electrode materials for next generation Li-ion Batteries."

Advisor: Sergio Brutti

Education

December 2018 **Master's degree in Sciences and Technologies of Industrial Chemistry**, University of Naples Federico II

Thesis: *Ab initio* study of oxygen electrocatalysis on Mn and Fe co-doped BaZrO₃: from bulk properties to surface reactions.

Advisor: Prof.ssa Ana Belén Muñoz García.
Co-Advisor: Prof. Michele Pavone.

Final grade: 110/110 cum laude.

March 2016 **Bachelor's degree in Industrial Chemistry**, University of Naples Federico II

Thesis: Proton Transport in BaZrO₃-based materials for solid oxide electrochemical cells.

Advisor: Prof.ssa Ana Belén Muñoz García.
Co-Advisor: Prof. Michele Pavone.

Scientific Publication

A.B. Muñoz-Garcia, M. Tuccillo and M. Pavone, Computational Design of cobalt-free mixed proton-electron conductors for solid oxide electrochemical cells, *J. Mater. Chem. A*, **5**, 11825–11833, (2017)

M. Tuccillo, O. Palmbo, M. Pavone, A.B. Muñoz-Garcia, A. Paolone and S. Brutti, Analysis of the phase stability of LiMO₂ layered oxides (M=Co, Mn, Ni), *Crystal*, **10 (6)**, 526, (2020)

A. Massaro, M. Tuccillo, M. Pavone and P.P. Prosini, Ab Initio Study of Li/Ni Doped Na_xMeO₂ Material for Na ion Batteries, *Journal of Energy and Power Technology*, **(3)**, 2, (2021)

A. Celeste, M. Tuccillo, A. Santoni, P. Reale, S. Brutti, and L. Silvestri, Exploring a Co-Free, Li-Rich Layered Oxide with Low Content of Nickel as a Positive Electrode for Li-ion Battery, *ACS Appl. Energy Mater.*, (2021)

M. Tuccillo, L. Mei, O. Palmbo, M. Pavone, A.B. Muñoz-Garcia, A. Paolone and S. Brutti, Replacement of Cobalt in Lithium-Rich Layered oxides by n-Doping: A DFT Study, *Appl. Sci.*, **11 (22)**, (2021)

C. Simari, M. Tuccillo, S. Brutti and I. Nicotera, Sodiated Nafion membranes for sodium metal aprotic batteries, *Electrochim. Acta*, 410, 139936, (2022)

M. Tuccillo, A. Costantini, A. Celeste, O. Palmbo, M. Pavone, A.B. Muñoz-García, A. Paolone and S. Brutti, NAl/Li Antisite Defects in the $\text{Li}_{1.2}\text{Ni}_{0.2}\text{Mn}_{0.6}\text{O}_2$ Li-Rich Layered Oxide: A DFT Study, *Crystal.*, 12 (5), (2022)

International Conference

XLIV Conference of the Physical Chemistry Division of the Italian Chemical Society (SCI), Naples, September 2016, poster presentation

XLVII Conference of the Physical Chemistry Division of the Italian Chemical Society (SCI), Rome, July 2019, poster presentation

European Materials Research Society 2019 Fall Meeting (E-MRS), Warsaw, September 2019, oral presentation

VI Conference of the Computational and Theoretical Chemistry Division (DCTC) of the Italian Chemical Society (SCI), Arcavacata di Rende, September 2019, oral presentation

Merck Young Chemists' Symposium 2019 organized by the Young Group of Italian Chemical Society (SCI), Rimini, November 2019, poster presentation

Nanoinnovation Conference & Exhibition 2020, Rome, September 2020, oral presentation

Workshop of the Physical Chemistry Division of the Italian Chemical Society (SCI), Rome, December 2020, oral presentation

European Materials Research Society 2021 Fall Meeting (E-MRS), September 2021, oral presentation

XXVII Conference of the Italian Chemical Society (SCI), Milan, September 2021, oral presentation

Research Experience

March 2022-July 2022

Borse di Mobilità Individuale all'estero per studenti di dottorato:

Project Title:

Influence of Oxygen release from Li-rich layered oxide materials (LRLO) Co-free investigated by On-Line Electrochemical Mass Spectrometry.

Group of Prof. Stefan Freunberger, Institute of Science and Technology (IST) Austria.

November 2021-February 2022

Tutor B2 in General and Inorganic Chemistry

Study Courses of the Faculty of Mathematical, Physical and Natural Sciences

2020-Now

PhD student, University of Rome "La Sapienza"

Aims: Study of novel positive electrode materials: synthesis, characterisation and electrochemical properties; structural and thermodynamic properties of mixed lithium and transition metal oxides, using ab initio calculations, in particular DFT+U method

- 2019-2020 **Researcher Fellow**, ISC-CNR (Rome)
Aims: Study of the structural and thermodynamic properties of mixed lithium and transition metal oxides, using ab initio calculations, in particular DFT+U method, in the project Silicon alloying anodes for energy dense batteries comprising lithium rich cathodes and ionic liquid electrolytes for safe high voltage performance (Si-DRIVE).
- 2017-2018 **Internship**, University of Naples Federico II
Aims: Study of the properties of perovskite BaZrO₃ co-doped with both Mn and Fe to evaluate whether this material presents mixed proton and electron conductive properties (MPEC) and good electrocatalytic capabilities towards oxygen reduction reaction (ORR) and oxygen evolution reaction (OER), for application as single phase electrode in proton-conducting solid oxide fuel and electrolyzer cells (PC-SOFC/EC), using ab initio calculations, in particular DFT+U method.
- 2015-2016 **Internship**, University of Naples Federico II
Aims: First principles investigation on derivatives of parent material BaZrO₃ (BZO), doped with transition metal oxides, namely Mn and Fe.

Personal Skills

- Language** Italian: mother tongue
English: (CEFR C1)
French: basic
- Software** Windows, Linux and Mac OS. Microsoft Office suite of programs for data collection and presentation. Gaussian and Vasp codes for computational modelling of molecules and materials, VESTA, GaussView for 3D visualization. LabView, Origin, MATLAB, CAD software. Python. GSAS II. XPS-Casa. VBA.
- Others** Data collection and analysis, problem solving and communication skills. 3D models and use of 3D printer.

La sottoscritta Tuccillo Mariarosaria, nata a Caserta il 29/01/1994, residente a Frattamaggiore (NA) in Via Cumana 7, a conoscenza di quanto prescritto dall'art. 76 del D.P.R. 28 dicembre 2000 n. 445, sulla responsabilità penale cui può andare incontro in caso di falsità in atti e di dichiarazioni mendaci, nonché di quanto prescritto dall'art. 75 del D.P.R. 28 dicembre 2000 n. 445, sulla decadenza dai benefici eventualmente conseguenti al provvedimento emanato sulla base di dichiarazioni non veritiere, ai sensi e per gli effetti del citato D.P.R. n. 445/2000 e sotto la propria personale responsabilità, dichiara che tutte le informazioni contenute nel curriculum vitae sono veritiere.

Data

22/04/2022

Firma

