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

April 2019 – October 2020

Research Fellow at Consiglio Nazionale di Ricerca – Istituto dei Sistemi Complessi (ISC-CNR)

Topic: SILICON ALLOYING ANODES FOR ENERGY DENSE BATTERIES COMPRISING LITHIUM RICH CATHODES AND IONIC LIQUID ELECTROLYTES FOR SAFE HIGH VOLTAGE PERFORMANCE (SI-DRIVE).

Advisor: Dr.ssa Annalisa Paolone, Dr.ssa Oriele Palumbo, Prof. Sergio Brutti, Prof. Michele Pavone.

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 $BaZrO_3$: 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 $BaZrO_3$-based materials for solid oxide electrochemical cells.

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

Scientific Publication

A.B. Muñoz-Garcìa, 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-Garcìa, A. Paolone and S. Brutti, Analysis of the phase stability of $LiMO_2$ 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_xMeO_2 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-Garcìa, A. Paolone and S. Brutti, Replacement of Cobalt in Lithium-Rich Layered oxides by n-Doping: A DFT Study, *Appl. Sci.*, ***11 (22)*****, (**2021)

International Conferences

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 & Exibithion 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

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

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 $BaZrO_3$ 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 $BaZrO_3$ (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.

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.