

Micaela Matta, PhD

Computational Materials Design

HOME Chicago, IL

MAIL matta.micaela@gmail.com

WEB <https://micaela-matta.github.io>

RESEARCH INTERESTS

organic (bio)-electronics, mechanical properties of molecular solids, design of materials and interfaces for organic photovoltaics, charge/exciton transport, molecular dynamics, (TD)-DFT, semi-empirical methods

SOFTWARE

lammps
NAMD
Gromacs
Tinker
ORCA
Gaussian09
QChem
ADF
MOPAC

EMPLOYMENT HISTORY

Mar 2017 – present

Postdoctoral Researcher @ **Northwestern University**

PI: **Prof. George Schatz**

Feb 2015 – Jan 2017

LabEx AMADEus Postdoctoral Researcher @ **Université de Bordeaux**

PI: **Prof. Luca Muccioli**

LANGUAGES

python
fortran
bash
tcl
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English
Italian
French
Spanish

EDUCATION

Jan 2012 – Apr 2015

PhD in Physical Chemistry @ **Università di Bologna**

PI: **Prof. Francesco Zerbetto**

Oct 2009 – Jun 2013

Diploma @ **Collegio Superiore dell'Università di Bologna**

Advanced multidisciplinary studies

Oct 2009 – Oct 2011

Master in Photochemistry and Molecular Materials @ **Università di Bologna**

PIs: **Prof. Luisa de Cola, Prof. Francesco Zerbetto**

March – June 2011

Erasmus Placement Fellowship @ **WWU Münster, Germany**

PI: **Prof. Luisa de Cola**

Oct 2006 – Oct 2009

Bachelor in Chemistry @ **Università di Sassari**

PUBLICATIONS

- 1) Swick, S.M.; Zhu, W.; **Matta, M.**; Aldrich, T.J.; Ortiz, R.P.; Kohlstedt, K.L.; Schatz, G.C.; Facchetti, A.; Melkonian, F. S.; Marks, T. J. Closely Packed, Low Reorganization Energy π -Extended Post-Fullerene Acceptors for Efficient Polymer Solar Cells, PNAS, *accepted*.
- 2) Gali, S. M.; **Matta, M.**; Lessard, B.H.; Castet, F.; Muccioli, L. Ambipolarity and Dimensionality of Charge Transport in Crystalline Group 14 Phthalocyanines: A Computational Study, J. Phys. Chem. C 2018, 122, 5, 2554–2563.
- 3) **Matta, M.**; Pereira, J. M.; Gali, S. M.; Thuau, D.; Olivier, Y.; Briseno, A.; Dufour, I.; Ayela, C.; Wantz, G.; Muccioli, L. Unusual electromechanical response in rubrene single crystals, Mater. Horizons 2018, 5, 41.
- 4) Álvarez-Asencio, R.; Moreno-Ramírez, J.; Pimentel, C.; Casado, S.; **Matta, M.**; Muccioli, L.; Jun Yoon, S.; Varghese, S.; Young Park, S.; Gierschner, J.; Gnecco, E.; Pina, C. M. Molecular-scale shear response of the organic semiconductor β -DBSCS(100) surface, Phys. Rev. B 2017, 96(11), 115422.
- 5) **Matta, M.**;^{*} Biscarini, F.; Zerbetto, F. Electric Field Promotes Pentacene Dimerization in Thin Film Transistors, J. Phys. Chem. C 2016, 120, 13942–13947.
- 6) Liscio, F.; Ferlauto, L.; **Matta, M.**; Pfattner, R.; Murgia, M.; Rovira, C.; Mas-Torrent, M.; Zerbetto, F.; Milita, S.; Biscarini, F. Changes of the Molecular Structure in Organic Thin Film Transistors during Operation, J. Phys. Chem. C 2015, 119, 15912–15918.
- 7) Toth, K.; Molloy, J. K.; **Matta, M.**; Heinrich, B.; Guillon, D.; Bergamini, G.; Zerbetto, F.; Donnio, B.; Ceroni, P.; Felder-Flesch, D. A strongly emitting liquid-crystalline derivative of Y3N@C80: bright and long-lived near-IR luminescence from a charge transfer state, Angew. Chem. Int. Ed. Engl. 2013, 52, 12303–12307.

AWARDS

2009 - 2012 Scholarship of Collegio Superiore dell'Università di Bologna
2010 - 2012 Regional scholarship for Sardinian students
2009 Università di Sassari award

TEACHING & MENTORING

@ Northwestern University	CHEM 171-0 Advanced General Chemistry 1 Substituting George Schatz in October 2018
	Graduate students: Matthew S. J. Kelley, Lauren E. Jones Undergraduates: Leighton Zhao
@ Université de Bordeaux	Theoretical Chemistry laboratory Master in Science, Technology, Health, AY 2015-2016
	Graduate students: Manoj S. Gali
@ Università di Bologna	Kinetics and Thermodynamics laboratory Bachelor in Chemistry, AYs 2012-2013, 2013-2014
	Properties of Molecular Materials laboratory Master in Chemistry, AY 2013-2014

CONFERENCES & SEMINARS

- 1) **Oral contribution** @ International Conference on Molecular Simulation, Oct 23-26, 2016 – Shanghai, China
- 2) **Poster** @ Second CCPBioSim/CCP5 Multiscale Modelling Conference Apr 13-15, 2016 – Manchester, UK
- 3) **Oral contribution** @ 7th European Symposium on Computing π -Conjugated Compounds, Feb 11-12, 2016 – Bordeaux, France (also part of the Organizing Committee)
- 4) **Oral contribution** @ 12th International Symposium on Functional π -Electron Systems (F π -12), Jul 19-24, 2015 – University of Washington, Seattle, USA
- 5) **Oral contribution** @ 6th European Symposium on Computing π -Conjugated Compounds, Feb 5-7, 2015 – Olomouc, Czech Republic
- 6) **Invited seminar** @ Institut des Sciences Moléculaires, Dec 10, 2014 – Bordeaux, France
- 7) **Oral contribution** @ XIV Società Chimica Italiana & Sigma-Aldrich Young Chemists Symposium, Oct 27-29, 2014 – Riccione, Italy
- 8) **Oral contribution** @ ETSF Young Researchers Meeting, May 12-16, 2014 – Roma, Italy