Micaela Matta, PhD

Royal Society Newton International Fellow

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RESEARCH INTERESTS

- Melanin-derived biocompatible semiconductors
- Organic bioelectronics, polymers for ionic/electronic transport
- Mechanical and charge transport properties of molecular solids
- Morphology-structure-charge transport in organic photovoltaics
- Python tools for computational chemistry

EMPLOYMENT HISTORY

Apr 2019 – present
Marie Skłodowska-Curie Fellow, Royal Society Newton International Fellow
University of Liverpool
Host: Prof. Alessandro Troisi

Mar 2017 – Feb 2019
Postdoctoral Researcher – **Northwestern University**
PI: Prof. George C. Schatz

Feb 2015 – Jan 2017
LabEx AMADEus Postdoctoral Researcher – **Université de Bordeaux**
PI: Prof. Luca Muccioli

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 – **University of Münster**
PI: Prof. Luisa de Cola

Oct 2006 – Oct 2009
Bachelor in Chemistry – **Università di Sassari**

TEACHING & MENTORING EXPERIENCE

University of Liverpool	**Mentoring:** Maryam Reisjalali, James Osborne*, Chloé Simha*
Northwestern University	**Mentoring:** Matthew S. J. Kelley, Laurel E. Jones, Leighton Zhao* **Teaching:** Guest lectures, CHEM 171-0 Advanced General Chemistry 1 (2018-2019)
Université de Bordeaux	**Mentoring:** Manoj S. Gali **Teaching:** Theoretical Chemistry Laboratory (2015-2016)
Università di Bologna	**Teaching:** Kinetics and Thermodynamics Laboratory (2012-2013, 2013-2014), Properties of Molecular Materials Laboratory (2013-2014)

* undergraduate students

MANUSCRIPTS IN PREPARATION

- **Matta, M.***; Wu, R.; Paulsen, B.; Schatz, G. C.; Rivnay, J. Trends in electrolyte behavior at the p(g2T-TT)-water interface, ***in preparation***.
- Gowers, R. J.; Chapman, C. T.; Schatz, G. C.; **Matta, M.*** kugupu: a software package for the characterization of dynamic molecular charge transport networks, ***in preparation***.
- **Matta, M.***; Pezzella, A.; Troisi, A. The hierarchical conformational space of DHICA oligomers: towards an accurate model of natural and synthetic eumelanins, ***in preparation***.

PEER-REVIEWED PUBLICATIONS

1) Wang, G.#; Swick, S.#; **Matta, M.#**; Mukherjee, S.; Strzalka, J.; Logsdon, J. L.; Fabiano, S.; Huang, W.; Aldrich, T.J.; Yang, T.; Timalsina, A.; Powers-Riggs, N.; Alzola, J.; Young, R. M., DeLongchamp, D. M.; Wasielewski, M. R.; Kohlstedt, K. L.; Schatz, G. C; Melkonian,F. S.; Facchetti, A.; Marks, T. J. Photovoltaic blend microstructure for high efficiency post-fullerene solar cells. To tilt or not to tilt?, ***J. Amer. Chem. Soc.*** **2019**,141 (34), 13410−13420.
2) Aldrich, T.J.; **Matta, M.***; Zhu, W.; Stern, C.; Schatz, G. C; Facchetti, A.; Melkonian,F. S.; Marks, T. J. Fluorination Effects on Indacenodithienothiophene Acceptor Packing and Electronic Structure, End-Group Redistribution, and Solar Cell Photovoltaic Response, ***J. Amer. Chem. Soc.*** **2019**, 141 (7), 3274−3287.
3) Pereira, M.; **Matta, M.**; Gali, M. S.; Ayela, C.; Hirsch, L.; Olivier, Y.; Muccioli, L.; Wantz, G. Application of rubrene air-gap transistors as sensitive MEMS physical sensors, ***ACS Appl. Mater. Interfaces*** **2018**, 10 (48), 41570−41577.
4) 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, ***Proc. Nat. Acad. Sci.*** **2018**, 115 (36), E8341-E8348.

5) 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.
6) **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.
7) 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.
8) **Matta, M.***; Biscarini, F.; Zerbetto, F. Electric Field Promotes Pentacene Dimerization in Thin Film Transistors, ***J. Phys. Chem. C*** **2016**, 120, 13942−13947.
9) 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.
10) 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.

#these authors contributed equally, *corresponding author.

AWARDS

- H2020 Marie Skłodowska-Curie Individual Fellowship (success rate ~ 14%)
- Royal Society Newton International Fellowship (success rate ~ 8%)
- Scholarship of Collegio Superiore dell'Università di Bologna (Oct 2009 - Oct 2011)
- Regional scholarship for excellent Sardinian students (2010, 2011, 2012)
- University of Sassari award (2009)

GRANT PORTFOLIO

- Google Summer of Code program – **$6500**
- Marie Skłodowska-Curie Individual Fellowship – **€212,933.76**
- Royal Society Newton International Fellowship – **£99,000.00**
- NumFOCUS Development Grant to Open Source Projects (MDAnalysis) – **$2,500.00**
- Workshop Organization Grant from McCormick School of Engineering and Weinberg College of Arts and Science – **$1,350.00**
- XSEDE Startup Allocation (2,500.0 GPU Hours) – **$700.00**
- Northwestern University Postdoc Professional Development Travel Grant – **$500.00**

- MRS Meeting Fall 2018 Postdoc Hardship Registration Grant – **$360.00**

SERVICE

- **Main organiser,** Royal Society Hooke Theo Murphy Meeting Proposal "Molecular scale challenges in bioelectronics" (submitted Sept 2019, success rate ~56%)
- **Reviewer,** The Journal of Physical Chemistry
- **Coordinator,** 500WomenScientists Liverpool pod
- **Mentor,** Google Summer of Code 2019 with MDAnalysis
- **Organizer,** NumFOCUS Workshop on MDAnalysis at Northwestern University (Nov 2018)
- **Subtask coordinator,** Argonne-Northwestern Solar Energy Research Center and Center for Light and Energy Activated Processes (Jan 2018 - Feb 2019)
- **Organizing committee,** 7th European Symposium on Computing π-Conjugated Compounds at Université de Bordeaux (Feb 2016)

DISSEMINATION AND OUTREACH

- **Volunteer,** Soapbox Science Chicago (2018)
- **Talk** "Mamma mia! Solar energy from spaghetti polymers", Wonder and Skepticism, Chicago (2018)

SOFTWARE DEVELOPMENT PROJECTS

- **MDAnalysis** (https://www.mdanalysis.org): open source software for analysis and post-processing of molecular dynamics simulations.
- **kugupu** (https://github.com/kugupu/kugupu): open source software for the characterization of charge transport networks in organic semiconductors.

SELECTED TALKS AND CONTRIBUTIONS

1. **Invited talk** (title tbd), Telluride Workshop "Organic Bioelectronics: Tackling the Mixed Conduction Challenge", Aug 3-7 2020 – Telluride, USA
2. **Seminar** (title tbd), Postdoc Seminar Series, School of Physical Sciences Research Forum, Nov 20 2019 – Liverpool, UK
3. **Seminar** (title tbd), Imperial College London (host: Prof. Jenny Nelson, Prof. Kim Jelfs), Nov 13 2019 – London, UK
4. **Invited talk** (title tbd), Max Planck Institute for Polymer Research (host: Prof. Denis Andrienko), Nov 5 2019 – Mainz, Germany
5. **Seminar** "Polymer semiconductors for organic (bio)electronics", Università di Napoli (host: Prof. Alessandro Pezzella), Oct 18 2019 – Naples, Italy

6. **Seminar** "Polymer semiconductors for organic (bio)electronics", Department of Electrical Engineering, University of Cambridge (host: Prof. George Malliaras), Jul 22, 2019 – Cambridge, UK
7. **Seminar** "Modeling materials for organic electronics" Institut des Sciences Moléculaires, Dec 10, 2014 – Bordeaux, France

1. **Oral contribution** "Charge transport networks in amorphous organic semiconductors ", ACS National Meeting Fall 2019, Aug 24-29 2019 – San Diego, USA
2. **Oral contribution** "Optimization of donors and acceptors for organic photovoltaics guided by molecular simulations", ACS National Meeting Fall 2019, Aug 24-29 2019 – San Diego, USA
3. **Oral contribution** "Optimization of donors and acceptors for organic photovoltaics guided by molecular simulations" 14th International Symposium on Functional π-Electron Systems (Fπ-14), Jun 2-7, 2019 – Berlin, Germany
4. **Selected oral contribution** "Design and Morphology Tuning of Novel Non-Fullerene Acceptors for Organic Photovoltaics" Computational Molecular Science 2019, Mar 26-29, 2019 – Warwick, UK
5. **Oral contribution** "Side Chain Engineering of Polymer Donors and Non-Fullerene Small Molecule Acceptors for Organic Photovoltaics" MRS Fall Meeting, Nov 20-25, 2018 – Boston, USA
6. **Oral contribution** "Rubrene single crystals under stress: clarifying strain-mobility trends" International Conference on Molecular Simulation, Oct 23-26, 2016 – Shanghai, China
7. **Oral contribution** "Rubrene single crystal air-gap transistors as highly sensitive mechano-electrical transducers" 7th European Symposium on Computing π-Conjugated Compounds, Feb 11-12, 2016 – Bordeaux, France
8. **Oral contribution** "Effect of the electric field on pentacene stability in OFETs" 12th International Symposium on Functional π-Electron Systems (Fπ-12), Jul 19-24, 2015 – University of Washington, Seattle, USA
9. **Oral contribution** "Exciton simulations: from liquid crystals to porphyrin-CNT aggregates" 6th European Symposium on Computing π-Conjugated Compounds, Feb 5-7, 2015 – Olomouc, Czech Republic
10. **Oral contribution** XIV Società Chimica Italiana & Sigma-Aldrich Young Chemists Symposium, Oct 27-29, 2014 – Riccione, Italy
11. **Oral contribution** ETSF Young Researchers Meeting, May 12-16, 2014 – Rome, Italy

1. **Poster** "Unraveling the conformational space and unique electronic properties of DHICA melanin" OrbItaly 2019, Oct 21-24, 2019 – Naples, Italy
2. **Poster** "Rubrene single crystal air-gap transistors as highly sensitive mechano-electrical transducers" Second CCPBioSim/CCP5 Multiscale Modelling Conference, Apr 13-15, 2016 – Manchester, UK

3. **Poster** "Electrolyte-polymer interactions in hydrated p(g2T-TT) interfaces", Asilomar Bioelectronics Symposium 2019, Sep 3-7 2019 – Asilomar, USA

REFERENCES

Prof. Francesco Zerbetto (**Master and PhD advisor**)
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Prof. Luisa De Cola (**Master project advisor**)
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