Micaela Matta, PhD

Marie Skłodowska-Curie Fellow

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RESEARCH INTERESTS

- Morphology and charge transport in organic semiconductors
- Structure-properties of eumelanin; eumelanin materials for bioelectronics
- Conducting polymers and materials for electronic and ionic transport

Employment History

Apr 2020 – present
Marie Skłodowska-Curie Fellow, **University of Liverpool**
H2020-MSCA-IF project BIOMOSAIC

Apr 2019 – March 2020
Royal Society Newton International Fellow, **University of Liverpool**
Research activity: eumelanin structure-properties; eumelanin-derived materials as biocompatible mixed conductors, morphology and ion percolation in conducting polymers for organic bioelectronics
Host: Prof. Alessandro Troisi

Mar 2017 – Feb 2019
Postdoctoral research associate, **Northwestern University**
Research activity: molecular dynamics simulations and electronic structure calculations; structure-properties of novel nonfullerene acceptors and polymer donors for organic solar cells; morphology and ion percolation in conducting polymers for organic bioelectronics.
PI: Prof. George C. Schatz

Feb 2015 – Jan 2017
LabEx AMADEus Postdoctoral research associate, **Université de Bordeaux**
Research activity: molecular dynamics simulations and electronic structure calculations; mechanical and charge transport properties of crystalline molecular semiconductors for actuators, sensors and functional interfaces.
PI: Prof. Luca Muccioli

Education

Jan 2012 – Apr 2015
PhD in Physical Chemistry, **Università di Bologna**
Research activity: electronic structure calculations; photophysical properties and self-organisation of molecular semiconductors (pentacene, dyes and fullerene cages) for organic photovoltaics and field effect transistors. Funding: iONE FP7 (€3.8M, 36 months).
PI: Prof. Francesco Zerbetto

Oct 2009 – Oct 2011
Master in Photochemistry and Molecular Materials, **Università di Bologna**
PIs: Prof. Luisa de Cola, Prof. Francesco Zerbetto

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

Grant Portfolio

- Marie Skłodowska-Curie Individual Fellowship – **€212,933.76**
- Royal Society Newton International Fellowship – **£99,000.00**
- Tier 2 Open Access Allocation (120,000.0 hours, HPC Midlands Plus) – **£1,104.00**
- Google Summer of Code 2019 program – **$6500**
- 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**

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)

Teaching and Mentoring

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 - Master in Chemistry 2015-2016
Università di Bologna	**Teaching:** Kinetics and Thermodynamics Laboratory - Bachelor in Chemistry 2012-2013, 2013-2014; Properties of Molecular Materials Laboratory - Master in Chemistry 2013-2014

Service

- **Main organiser,** Royal Society Hooke Theo Murphy Meeting Proposal "Molecular scale challenges in bioelectronics" (not funded)
- **Reviewer,** The Journal of Physical Chemistry, Physical Review Materials, Chemistry Select, ACS Applied Materials and Interfaces
- **Coordinator,** 500WomenScientists Liverpool pod
- **Mentor,** Google Summer of Code 2019 with MDAnalysis
- **Organizer,** NumFOCUS Workshop on MDAnalysis (Nov 2018)

- **Subtask coordinator,** Argonne-Northwestern Solar Energy Research Center, 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

- **Invited talk "**Building STEM community across continents: my academic journey" - Liverpool School of Physical Sciences Lunch and Learn (Nov 2020)
- **Talk** "Bringing melanin's dark secrets to light: towards next-gen nanomedicine" - Pint of Science Liverpool 2020 (postponed to May 2021)
- **Talks** "My scientific journey", secondary school outreach/science communication events - Alghero, Italy (Dec 2019)
- **Volunteer,** SkypeAScientist (2019/2020) and Soapbox Science Chicago (2018)
- **Talk** "Mamma mia! Solar energy from spaghetti polymers", Wonder and Skepticism café scientifique, Chicago, IL (July 2018)

Active Collaborators

- Jonathan Rivnay, Northwestern University
- Iain McCulloch, University of Oxford/KAUST
- Simone Fabiano, Linköping University
- Alessandro Pezzella, Università di Napoli

Selected Talks and Contributions

1. **Invited talk** (title tbd), Telluride Workshop "Organic Bioelectronics: Tackling the Mixed Conduction Challenge", TSRC -Telluride, USA (cancelled due to COVID-19)
2. **Seminar** "Polymer semiconductors for organic electronics and bioelectronics", Postdoc Seminar Series, School of Physical Sciences Research Forum, Nov 20 2019 – Liverpool, UK
3. **Seminar** "Polymer semiconductors for organic electronics and bioelectronics", Imperial College London (host: Prof. Kim Jelfs), Nov 13 2019 – London, UK
4. **Seminar** "Polymer semiconductors for organic electronics and bioelectronics", MPIP Mainz (host: Prof. Denis Andrienko), Nov 5 2019 – Mainz, Germany
5. **Seminar** "Polymer semiconductors for organic (bio)electronics", Università di Napoli (host: Dr. 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** "Eumelanin: a biocompatible mixed conductor", E-MRS 2020 Spring Meeting (cancelled due to COVID-19)
2. **Oral contribution** "Eumelanin: a biocompatible mixed conductor", Faraday joint interest group conference 2020, University of Sheffield – Sheffield, UK (postponed to 2021)

3. **Oral contribution** "Charge transport networks in amorphous organic semiconductors ", ACS National Meeting Fall 2019, Aug 24-29 2019 – San Diego, USA
4. **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
5. **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
6. **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
7. **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
8. **Oral contribution** "Rubrene single crystals under stress: clarifying strain-mobility trends" International Conference on Molecular Simulation, Oct 23-26, 2016 – Shanghai, China
9. **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
10. **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
11. **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
12. **Oral contribution** XIV Società Chimica Italiana & Sigma-Aldrich Young Chemists Symposium, Oct 27-29, 2014 – Riccione, Italy
13. **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

Peer-reviewed publications

# = these authors contributed equally; * = corresponding author.

1. **Matta, M.;*** Wu, R.; Paulsen, B. D.; Petty, A. J.; Sheelamanthula, R.; McCulloch, I.; Schatz, G. C.; Rivnay, J. Ion Coordination and Chelation in a Glycolated Polymer Semiconductor: Molecular Dynamics and X-Ray Fluorescence Study, DOI:10.26434/chemrxiv.12264308 and ***Chem. Mater. 2020***, 32 (17), 7301–7308.

2. Moser, M.; Savagian, L.; Savva, A.; **Matta, M.;** Ponder, J.; Hidalgo Castillo, T.; Ohayon, D.; Hallani, R.; Reisjalali, M.; Troisi, A.; Wadsworth, A.; Reynolds, J.; Inal, S.; McCulloch, I. Ethylene Glycol Based Side Chain Length Engineering in Polythiophenes and its Impact on Organic Electrochemical Transistor Performance, ***Chem. Mater. 2020***, 32 (15), 6618–6628.
3. **Matta, M.;*** Pezzella, A.; Troisi, A. Relation Between Local Structure, Electric Dipole and Charge Carrier Dynamics in DHICA Melanin, a Model for Biocompatible Semiconductors, ***J. Phys. Chem. Lett.* 2020**, 11 (3), 1045–1051.
4. 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.
5. 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.
6. 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.
7. 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.
8. 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.
9. **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.
10. 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.
11. **Matta, M.;*** Biscarini, F.; Zerbetto, F. Electric Field Promotes Pentacene Dimerization in Thin Film Transistors, ***J. Phys. Chem. C* 2016**, 120, 13942–13947.
12. 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.
13. 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.