Stefano Falletta

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Homepage, LinkedIn, Google Scholar, GitHub, GitLab

Research Experience

03/2023 – (present) **Postdoctoral Fellow**, *Harvard University*, USA.
Advisor: Prof. B. Kozinsky.
- Developed a machine-learning framework for unified differentiable learning of electric enthalpy and dielectric properties with exact physical constraints. Implementation in the equivariant neural network Allegro. Applied the method to study vibrational and dielectric properties of solids.
- Improved the machine-learning exchange functional CIDER to address the band gap problem through learning of the single-particle energy levels. Applied the method to study band gaps of molecules, and formation energies of polarons.

2018 – 2023 (4 yr 5 mo) **Doctoral Researcher**, *EPFL*, Switzerland.
Advisor: Prof. A. Pasquarello.
- Developed finite-size corrections of defect energy levels involving ionic polarization. Applied the method to calculate accurate vertical transitions energies of defets and to enforce the piecewise-linearity condition when studying polarons.
- Developed a unified theoretical formulation encompassing one-body and many-body forms of electron self-interaction, and conferred superiority to the many-body notion of self-interaction. Applied the method to determine formation energies of polarons in solids.
- Developed the γDFT and the μDFT semilocal functionals for localizing polarons and addressing the electron self-interaction. Included in the code QuantumESPRESSO two new modules (`sic.f90`, `scissor.f90`) and related interface to `pw.x` (main changes). Applied the method to study formation energies and transport properties of polarons in solids.
- Developed a one-shot approach for constructing nonempirical hybrid functionals and range-separated hybrid functionals. Implemented the method in the code QuantumESPRESSO.
- Studied the band alignment at semiconductor-water interfaces for photocatalytic water splitting.

2018 (2 mo) **Research Scholar**, *Fermi National Accelerator Laboratory*, USA.
Advisor: Prof. E. Barzi.
- Optimized the fabrication of superconducting Nb_3Sn samples.

2018 (6 mo) **Research Scholar**, *École Polytechnique*, France.
Advisor: Prof. S. Biermann.
- Studied the electronic, structural and magnetic properties of honeycomb iridates.

2017 (2 mo) **Research Scholar**, *Fermi National Accelerator Laboratory*, USA.
Advisor: Prof. E. Barzi.
- Defined the experimental procedure to fabricate superconducting Nb_3Sn samples.

Education

2018 – 2023 **Ph.D. in Physics**, *EPFL*, Switzerland.
Computational condensed matter physics, electronic structure, materials science.
Thesis: "Self-Interaction and Polarons in Density Functional Theory".

2016 – 2018 **M.Sc. in Physics of Complex Systems**, *Politecnico di Torino & Université Paris Sud*, Italy, France.
GPA: Summa cum laude (29.82/30.00). Joint double degree.

2016 – 2018 **M.Sc. in Mathematical Engineering**, *Politecnico di Milano*, Italy.
GPA: Summa cum laude.

2016 – 2018 **Diploma in Business Management and Entrepreneurship**, *Alta Scuola Politecnica*, Italy.
Honors program for top 150 students from *Politecnico di Torino* and *Politecnico di Milano*.

2013 – 2016 **B.Sc. in Physics Engineering**, *Politecnico di Torino*, Italy.
GPA: Summa cum laude (29.91/30.00).

Awards

2023 **Physics Doctoral Thesis Award**, *EPFL*, Switzerland.

2023 **Doctoral Program Thesis Distinction Award**, *EPFL*, Switzerland.

2023 **Postdoc Mobility Fellowship**, *Swiss National Science Foundation*, Switzerland, start date: 03/2024.

2022 **Poster Award**, *Psi-k*, Switzerland.

2022 **Coffee with Max Planck Award**, *Max Planck Society*, Germany.

2017 **International Master's Scholarship Paris Saclay**, *Université Paris Saclay*, France.

Leadership Experiences

2022 **Organizer of "First-Principles Modeling of Defects in Solids"**, *ETHZ*, Switzerland.
Workshop with 85 participants and 15 international speakers (*website*). Raised funding of 40'000 CHF.

2019 – 2022 **Organizer of "Marvel Junior Seminars"**, *EPFL*, Switzerland.
Monthly seminars, each with 2 speakers and around 50 participants.

2019 – 2022 **President of PolyPhys Association**, *EPFL*, Switzerland.
Association of *EPFL* doctoral students in Physics.

2020 – 2021 **PhD Student Representative**, *EPFL*, Switzerland.
Representative of the PhD students of the *EPFL* doctoral school in Physics.

2021 **Member of the Excellence Committee for the EPFLglobalLeaders programme**, *EPFL*.
Observer of the selection process for the EPFLglobalLeaders program.

2019 **Organizer of "Advanced Electronic Structure Methods in Condensed Matter Physics"**, *EPFL*, Switzerland.
Summer school with 120 participants and 15 international speakers (*website*). Raised funding of 40'000 CHF.

Selected Publications

2024 **S. Falletta***, A. Cepellotti, C. W. Tan, A. Johansson, A. Musaelian, C. J. Owen, and B. Kozinsky, *Unified Differentiable Learning of the Electric Enthalpy and Dielectric Properties with Exact Physical Constraints*, arXiv:2403.17207 (2024).

K. Bystrom, **S. Falletta**, B. Kozinsky, *Addressing the Band Gap Problem with a Machine-Learned Exchange Functional*, arXiv:2403.17002v2 (2024).

S. Falletta*, A. Pasquarello, *Nonempirical semilocal density functionals for correcting the self-interaction of polaronic states*, *J. Appl. Phys. 135, 13 (2024)*.

2023 **S. Falletta***, A. Pasquarello, *Polaron hopping through piecewise-linear functionals*, Phys. Rev. B 107, 205125 (2023).

B. Dou, **S. Falletta**, J. Neugebauer, C. Freysoldt, X. Zhang, S. Wei, *Chemical trend of nonradiative recombination in Cu(In,Ga)Se_2 alloys*, Phys. Rev. Appl. 19, 054054 (2023).

J. Yang, **S. Falletta**, A. Pasquarello, *Range-separated hybrid functionals for accurate band gap prediction*, npj Comput. Mater. 9(1), 108 (2023).

2022 **S. Falletta***, A. Pasquarello, *Hubbard U through polaronic defect states*, npj Comput. Mater. 8(1), 263 (2022).

S. Falletta*, A. Pasquarello, *Many-Body Self-Interaction and Polarons*, Phys. Rev. Lett. 129, 126401 (2022).

S. Falletta*, A. Pasquarello, *Polarons free from many-body self-interaction in density functional theory*, Phys. Rev. B, 106, 125119 (2022).

J. Yang, **S. Falletta**, A. Pasquarello, *One-shot approach for enforcing piecewise linearity on hybrid functionals: application to band gap predictions*, J. Phys. Chem. Lett. 13(13), 3066-3071 (2022).

2020 **S. Falletta***, J. Wiktor, A. Pasquarello, *Finite-size corrections of defect energy levels involving ionic polarization*, Phys. Rev. B, 102(4), 041115 (2022).

S. Falletta*, P. Gono, Z. Guo, S. Kampouri, K. Stylianou, A. Pasquarello, *Unraveling the synergy between metal-organic frameworks and co-catalysts in photocatalytic water splitting*, *J. Mater. Chem. A*, 8 (39), 20493-20502 (2020).

N. Österbacka, P. Erhart, **S. Falletta**, A. Pasquarello, J. Wiktor, *Small electron polarons in $CsPbBr_3$: competition between electron localization and delocalization*, Chem. Mater. 32 (19), 8393-8400 (2020).