

Curriculum vitae et studiorum

Anna Piras

annapiras7@gmail.com • anna.pirasmanca@pec.it • +39-345-6917928

ORCID iD: 0000-0002-1528-8874

Citizenship: Italy

Research interests

Computational Chemistry, Physical Organic Chemistry, Non-covalent Interactions, Carbon-Based Materials, Scientific Software Development

Methods

Density Functional Theory, Metadynamics, Symmetry Adapted Perturbation Theory, Time-Dependent Density Functional Theory, Multireference Methods, Montecarlo Methods, Multiscale Simulations, Molecular Dynamics

Employment

01 August
2024 – present

**Institute for the Chemistry of Organometallic compounds,
National Research Council (CNR-ICCOM) – Pisa, Italy**

Research associate

Project: SPOKE 11 “Innovative Materials and Lightweighting; task 6.1 “Materials development”

Topic: “Studio teorico-sperimentale di sistemi termochimici ad adsorbimento per il recupero e l’accumulo dell’energia termica”

01 April 2024
– 31 July 2024

**Institute for the Chemistry of Organometallic compounds,
National Research Council (CNR-ICCOM) – Pisa, Italy**

Research associate

Project: “Centre for HPC, Big Data and Quantum Computing – HPC” (PRR.AP001.004)

Topic: “Accelerating the pace of the energy transition through simulation-guided discovery of advanced green materials”

Education

- October 2019 – March 2024 **Heidelberg Institute for Theoretical Studies, Heidelberg University** – Heidelberg, Germany
PhD in Computational Chemistry *cum laude*
Thesis title: "Predicting Adsorbent and Electronic Properties of Graphene-Based Materials"
Supervisor: Dr. Ganna Gryn'ova
- 2017 – 2019 **Università di Bologna** – Bologna, Italy
MA in Chemistry, curriculum Synthetic Methodologies and Bio-Organic Chemistry
Final grade: 110/110 *cum laude*
Thesis title: "Computational investigations of organic reactions catalysed by graphene oxide"
Supervisor: Prof. Andrea Bottoni
- 2014 – 2017 **Università di Bologna** – Bologna, Italy
BA in Chemistry
Final grade: 108/110
Thesis title: "Determination of the structure and the dynamic of the gG'T conformer of N-methyl-2-aminoethanol in gas phase through microwave spectroscopy in Fourier transform"
Supervisor: Prof. Sonia Melandri

Awards

- 2021 HITS Award 2021 (Heidelberg Institute for Theoretical Studies)
for the outstanding engagement in several committees to improve various aspects of work and social life at HITS.
- 2014 Bronze Medal at the National Math Olympics (Unione Matematica Italiana)

Publications

- 2025 **A set of Quantum–Mechanically Derived Force Fields for Natural and Synthetic Retinal Photoswitches**
Razan Daoud, Simone Veglianti, Anna Piras, Abderrahmane Semmeq, Giacomo Prampolini and Daniele Padula
preprint 2025.
<https://doi.org/10.26434/chemrxiv-2025-chsf0>
- JOYCE3.0: A General Protocol for the Specific Parametrization of Accurate Intramolecular Quantum Mechanically Derived Force Fields**
Samuele Giannini, Pablo M. Martinez, Abderrahmane Semmeq, J. Pablo Galvez, Anna Piras, Alessandro Landi, Daniele Padula, J.G. Vilhena, Javier Cerezo and Giacomo Prampolini
Journal of Chemical Theory and Computation, 2025.
<https://doi.org/10.1021/acs.jctc.5c00010>
- 2023 **CO₂ on Graphene: Benchmarking Computational Approaches to Non-covalent Interactions**
Christopher Ehlert, Anna Piras, and Ganna Gryn'ova
ACS Omega 2023.
<https://doi.org/10.1021/acsomega.3c03251>
- Metal-Free Molecular Catalysts for the Oxygen Reduction Reaction: Electron Affinity as an Activity Descriptor**
Christopher Ehlert, Anna Piras, Juliette Schleicher, and Ganna Gryn'ova
J. Phys. Chem. Lett. 2023, 14, 2, 476–480.
<https://doi.org/10.1021/acs.jpcclett.2c03481>
- 2021 **Sensing and sensitivity: Computational chemistry of graphene-based sensors**
Anna Piras, Christopher Ehlert and Ganna Gryn'ova
WIREs Computational Molecular Science e1526.
<https://doi.org/10.1002/wcms.1526>
- 2018 **Rotational Spectrum and Conformational Analysis of N-Methyl-2-Aminoethanol: Insights into the Shape of Adrenergic Neurotransmitters**
Camilla Calabrese, Assimo Maris, Luca Evangelisti, Anna Piras, Valentina Paravicini and Sonia Melandri
Frontiers in Chemistry 2018, 6, 25.
<https://doi.org/10.3389/fchem.2018.00025>

Talks, workshops and posters

- February 2025 Contributed talk: "Development of QM-derived force-fields for small molecules adsorbed in carbon-based materials"
15th Symposium on Computing π -Conjugated Compounds, Siena, Italy
- January 2025 Accepted attendance to the workshop:
Advanced force fields in multiscale approaches to computational spectroscopy, Paris, France
- September 2024 Poster: "Development of QM-derived force-fields for the study of gas molecules adsorbed on carbon-based materials"
Challenges in Chemical Sensing with Graphene Derivatives and 2D materials (SENSE), San Sebastian, Spain
- June 2023 Poster: "Predicting adsorbent and electronic properties of nanographenes"
17TH INTERNATIONAL CONGRESS OF QUANTUM CHEMISTRY, Bratislava, Slovakia
- June 2022 Contributed talk: "Nitroaromatic pollutants on graphene: from physisorption to redox properties"
9th Young Scientists Workshop on Theoretical Chemistry and Computational Modelling, Vigo, Spain
- June 2022 Poster: "Nitroaromatic pollutants on graphene: from physisorption to redox properties"
12th Congress on Electronic Structure Principles and Applications, Vigo, Spain
- September 2021 Poster: "How can we simulate the detection of nitroaromatic contaminants by graphene-based sensors?"
18th European Symposium on Organic Reactivity (online)
- September 2021 Poster: "How can we simulate the detection of nitroaromatic contaminants by graphene-based sensors?"
Chem2DMat COncference (online)
- March 2021 Seminar talk: "How can we predict the performance of graphene-based sensors?"
Group of Prof. Hutter, University of Zurich
- October 2020 Poster: "The law of attraction: computational insights into the role of non-covalent interactions in graphene-based sensing"
Graphene2020 (online)

Other activities

Member of the Sustainability Committee at the Heidelberg Institute for Theoretical Studies

Member of the Diversity Committee at the Heidelberg Institute for Theoretical Studies

Staff Representative for the Computational Carbon Chemistry at the Heidelberg Institute for Theoretical Studies

February 2021 Curator of the RealScientists Nano Twitter profile

February 2021 Guest at the Under the Microscope Podcast <https://thesciencetalk.com/anna-piras/>

Technical skills

Operative Systems

Windows, Linux Ubuntu

Programming languages

Proficient in Python, including Matplotlib and Atomic Simulation Environment

Expert knowledge of Fortran Basic knowledge of Markdown

Software

Scientific software: Gromacs, Gaussian, PSI4, Orca, Joyce, QuantumEspresso, RASPA, xtb, ADF, DFTB+

Visualization software: Chimera, Avogadro, VMD, Gaussview, VESTA, Chemdraw

Other: \LaTeX , Microsoft Office package, Grace, Inkscape, Gitlab

Languages

Italian (native), English (fluent), German (intermediate), French (Intermediate)