



## Former Group Members

### ***Péter Szabó***

Position: Post-Doc

Years: 2019-2022

Topic: Fundamental Apects of Molecular Forces

Current position: KU Leuven

### ***Martin Stöhr***

Position: Ph.D. Student, Post-Doc

Years: 2016-2021

Topic: Long-Range Interactions for Biomolecular Systems

Current position: Post-Doc, Stanford

### ***Anirban Mondal***

Position: Post-Doc

Years: 2021

Topic: Machine Learning in Condensed Phase

Current position: Assistant Professor, Indian Institute of Technology, Gandhinagar

### ***Swastika Banerjee***

Position: Post-Doc

Years: 2021-2022

Topic: Role of Non-Local Many-Body Dispersion Interactions on Materials' Properties

Current position: Assistant Professor, Department of Chemistry, Indian Institute of Technology, Roorke

### ***Ali Asghar Hakami Zanjani***

Position: Ph.D. Student

Years: 2015-2019

Topic: Thermodynamics and Aggregation Kinetics of Lysozyme-Derived Peptides

Current position: Post-Doc, University of Southern Denmark

### ***Katerine Saleme Ruiz***

Position: Post-Doc

Years: 2017-2019

Topic: Many-Body Dispersion Interactions in Atomic Chains

Current position: Research Facilitator, University of Luxembourg

### ***Somayeh Khazaei***

Position: Post-Doc

Years: 2018-2020

Topic: Many-Body Interactions in Solid States

### ***Farnaz Heidar-Zadeh***

Position: Post-Doc

Years: 2017-2019

Topic: Designing new machine learning methods for chemical properties

Current Position: Associate Professor, McMaster University

### ***Dennis Barton***

Position: Post-Doc

Years: 2017-2019

Topic: Assessment of precision and reproducibility of vdW dispersion methods in electronic structure calculations

### ***Yasmine Al-Hamdani***

Position: Post-Doc

Years: 2017-2019

Topic: Quantum chemical benchmarking interaction energies through Quantum Monte Carlo

Current Position: Post-Doc at University of Zurich

### ***Johannes Hoja***

Position: PhD Student

Years: 2014-2018

Topic: Crystal Structure Predictions from First-Principle Calculations

Current Position: Tenure Track, University of Graz (Austria)

### ***Mainak Sadhukhan***

Position: Post-Doc

Years: 2016-2018

Topic: van der Waals interactions beyond dipole approximations

Current Position: Assistant Professor, Department of Chemistry, IIT Kanpur

### ***Jan Hermann***

Position: PhD Student

Years: 2013-2017

Topic: Many Body Methods

Current Position: Senior researcher, Microsoft Research Center, Berlin

***Guo-Xu Zhang***

Position: PhD Student

Years: 2010-2014

Topic: van der Waals in solids

Current Position: Associate Professor at HIT (Harbin Institute of Technology China)

***Javier Camarillo-Cisneros***

Position: PhD Visitor

Years: 2011-2014

Topic: Adsorption on stepped surfaces

Current Position: Researcher at Cinvestav, Chihuahua (Mexico)

***Xiaofei Liu***

Position: PhD Visitor

Years: 2016-2018

Topic: Metal-organic networks

Current Position: Associate Professor at Nanjing University of Aeronautics and Astronautics, China

***Victor Ruiz***

Position: PhD Student

Years: 2011-2016

Topic: van der Waals in Interfaces

Current Position: Research staff member at Helmholtz, Berlin

***Vivekanand Gobre***

Position: PhD Student

Years: 2011-2016

Topic: Electronic Structure Methods

Current Position: Assistant Professor in Pune, India

***Nicola Ferri***

Position: PhD Student

Years: 2011-2016

Topic: van der Waals and electronic properties

Current Position: IT in Milan, Italy

***Wei Liu***

Position: Post-Doc

Years: 2010-2014

Topic: Catalysis, interfaces

Current Position: Full Professor in Nanjing University of Science and Technology, China

***Wang Gao***

Position: Post-Doc

Years: 2013-2015

Topic: Defects, friction

Current Position: Professor at Jilin University, China

***Alberto Ambrosetti***

Position: Post-Doc

Years: 2012-2014

Topic: Many-body methods

Current Position: Professor at University of Padova, Italy

***Katja Hansen***

Position: Post-Doc

Years: 2012-2013

Topic: Machine learning

Current Position: Manager in 3M, Germany

***Anthony Reilly***

Position: Post-Doc

Years: 2012-2013

Topic: Molecular crystals

Current Position: Professor at City University Dublin

***Mausumi Chattopadhyaya***

Position: Post-Doc

Years: 2014-2017

Topic: Wetting

Current Position: Assistant Professor in Calcutta, India

***Fairoja Cheenicode-Kabeer***

Position: Post-Doc

Years: 2015-2017

Topic: Catalysis

Current Position: Post-Doc in Sweden

***Gionni Marchetti***

Position: Post-Doc

Years: 2014-2016

Topic: Machine learning

Topic: Machine Learning  
Current Position: Post-Doc in Riga

### ***Limin Zheng***

Position: Post-Doc  
Years: 2015-2016  
Topic: Nuclear quantum effects  
Current Position: Visiting Professor

### ***Andrii Kleschonok***

Position: Post-Doc  
Years: 2016-2018  
Current Position: Data Scientist at VW Labs, Germany

### ***Majid Mortazvi***

Position: Post-Doc  
Years: 2016-2018  
Current Position: Data Scientist at Siemens, Germany

### ***Huziel Saucedo***

Position: Post-Doc  
Years: 2017-2022  
Topic: Machine learned force fields  
Current Position: Assistant Professor, Instituto de Física, Universidad Nacional Autonoma de Mexico

### ***Niccolò Gentile***

Position: PhD Student  
Years: --  
Current Position: --

### ***Mario Galante***

Position: Post-Doc  
Years: 2019-2023  
Topic: van der Waals interactions, Density functional theory  
Current Position: Postdoc, Arizona State University

### ***Leonardo Medrano Sandomas***

Position: Post-Doc  
Years: 2019-2024  
Topic: Machine learning methods for understanding the chemical space of molecular systems  
Current Position: Research associate, TU Dresden, Germany

### ***Carolín Müller***

Position: Post-Doc  
Years: 2021-2024  
Topic: Theoretical Chemistry, Photochemistry  
Current Position: Run.-Prof. for the Theory of Electronically Excited States at FAU Erlangen-Nürnberg, Germany

### ***Jorge Alfonso Charry Martinez***

Position: Post-Doc, PhD.  
Years: 2023-2024, 2019-2013  
Topic: Positronic and positronium chemistry

### ***Gregory Cordeiro Fonseca***

Position: Post-Doc, PhD  
Years: 2023-2024, 2019-2023  
Topic: Machine Learning Force Fields Under the Microscope: Stability, Reliability, and Performance Analysis

### ***Matej Ditte***

Position: Post-Doc, PhD  
Years: 2023-2024, 2019-2023  
Topic: Molecules in Environments: Towards Systematic Quantum Embedding of Electrons and Drude Oscillators

### ***Szabolcs Goger***

Position: Post-Doc, PhD  
Years: 2023-2024, 2019-2023  
Topic: Development of Practical Non-Local Many-Body Polarization Functionals

### ***Dmitry Fedorov***

Position: Research Scientist  
Years: 2016-2024  
Topic: Theoretical Chemical Physics, Solid State Theory, First-Principles Calculations, Spintronics  
Current Position: Research Scientist Skolkovo Institute of Science and Technology, Russia