Dr. Jingjing Shao

jingjingshao@zedat.fu-berlin.de LinkedIn: jingjing-shao-38709a201

Skills

Quantum Chemistry	ab-initio DFT, Electronic structures, NEGF transport properties, Local current analysis, Many-body Green's function (GW approximation), Optical properties (RPA/TDDFT/BSE)
Research	Computational Modelling, Method Implementation, Transition state search
Tools	Python, Pandas, Pytorch, RDKt, deepChem, Matplotlib, Microsoft office, Linux, LaTeX, INKSCAPE, VESTA
Communication	Chinese (native), German (fluent), English (fluent)

Working Experience and Internships

Expert of Computational Chemistry **Oct 2022 — Present**
Covestro *Shanghai, China*

- Computational simulation of industrial relevant chemical reactions
- Implementing automatic workflow for quantum simulation
- Management of global collaborative research project
- Organization of regional global Townhall

Consultant **April 2022 — Sept 2022**
ADWEKO *Remote, Germany*

- Development of data management tool via SAP HANA WebIDE
- First experience in creating SQL databases

Doctoral/Postdoctoral Researcher **July 2018 — March 2022**
Freie Universität Berlin *Berlin, Germany*

- Scientific project management
- Computational simulation using VASP/GPAW/Gaussian/ASE/TURBOMOLE/Orca/Psi4/PySCF
- Scientific data analysis/ Scientific writing
- Supervision of master students

Teaching Assistant **Sept 2018 – March 2022**
Freie Universität Berlin *Berlin, Germany*

- Quantum Chemistry Analytical/Computational (Online) Tutorial
- Physical Chemistry Laboratory Assistant
- Atombau und Chemische Bindung Tutorial (In German)

Research Internship **Sept 2015 — Feb 2016**
Max-Planck-Institute *Potsdam, Germany*

- Organic synthesis of hydantoin derivatives via flow chemistry
- Laboratory equipment building
- High-Performance Liquid Chromatography (HPLC)/ Chromatography/ Characterization

Research Internship **Mar 2015 — June 2015**
Bayer Pharma AG *Berlin, Germany*

- Introducing flow chemistry synthesis
- Photosynthesis via flow chemistry

Education

Doctor Rerum Naturalium (Dr. rer. nat. - magna cum laude), *Freie Universität Berlin* July 2018- Sept 2021
Thesis: Electronic and Transport Properties of Carbon Based Materials
Supervisor: Prof. Dr. Beate Paulus

Master of Science, Chemistry (GPA: 3.7/4.0), *Freie Universität Berlin* Feb 2016- June 2018
Thesis: Theoretical Investigations on Graphene Antidot Lattices on Substrates
Supervisors: Prof. Dr. Beate Paulus & Prof. PhD. Jean Christophe Tremblay

Bachelor of Science, Chemistry, *Freie Universität Berlin* Sept 2012- Feb 2016
Thesis: Multiphase Synthesis of Hydantoins in Flow
Supervisor: Prof. Dr. Peter H. Seeberger (Max-Planck-Institute)

Activities and Scholarship

Shanghai Jiaotong University/Infineon Summer School 2021, Research Presentation Nov/Aug 2021
European Summer School in Quantum Chemistry, Poster Presentation, Torre Normanna, Italy (80 Students / 2 Years) Sept 2019
Nanoscale Focus Area 10,000 Euro Scholarship July 2018

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Publications

Studies on the local structure of the F/OH-site in topaz by MAS NMR and Raman spectroscopy

- *Anselm Loges, Gudrun Scholz, Nader De Sousa Amadeu, **Jingjing Shao**, Jeremy Fuller, Beate Paulus, Franziska Emmerling, Thomas Braun and Timm John*
- *Preprint DOI:10.13140/RG.2.2.13465.29286*

Edge Effect in Electronic and Transport Properties of 1D Fluorinated Graphene Materials

- ***Jingjing Shao**** *and Beate Paulus*
- *Nanomaterials 2022, 12(1), 125*

Electronic and Transport Properties of Carbon Based Materials

- ***Jingjing Shao***
- *Refubium FU Berlin 2021, 11*

Understanding Charge Transport in Triarylmethyl-Based Spintronic Nanodevices

- ***Jingjing Shao**, Isaac Alcón Rovira, Beate Paulus and Jean Christophe Tremblay**
- *J. Phys. Chem. C 2021, 125, 46, 25624–25633*

Conformational Control Over π-conjugated Electron Pairing in 1D Organic Polymers

- *Isaac Alcón Rovira*, **Jingjing Shao**, Jean Christophe Tremblay and Beate Paulus*
- *RSC Adv., 2021,11, 20498-20506*

Local Current Analysis on Defective ZGNRs Devices for Biosensor Material Applications

- ***Jingjing Shao***, Beate Paulus and Jean Christophe Tremblay**
- *J. Comp. Chem. 2021*

Electronic and Optical Properties of Fluorinated Graphene within Many-Body Green's Function Framework

- *Kangli Wang, **Jingjing Shao**** *and Beate Paulus*
- *J. Chem. Phys. 154, 2021, 104705*

Metal-Assisted and Solvent-Mediated Synthesis of Two-Dimensional Triazine Structures on Gram Scale

- *Abbas Faghani, Mohammad Fardin Gholami, Matthias Trunk, Johannes Müller, Pradip Pachfule, Sarah Vogl, Ievgen Donskyi, Mingjun Li, Philip Nickl, **Jingjing Shao**, Michael R. S. Huang, Wolfgang E. S. Unger, Raul Arenal, Christoph T. Koch, Beate Paulus, Jürgen P. Rabe, Arne Thomas*, Rainer Haag, and Mohsen Adeli*
- *J. Am. Chem. Soc. 2020, 142, 30, 12976–12986*

Electronic Current Mapping of Transport through Defective Zigzag Graphene Nanoribbons

- ***Jingjing Shao***, Vincent Pohl, Lukas Eugen Marsoner Steinkasserer, Beate Paulus and Jean Christophe Tremblay**
- *J. Phys. Chem. C 2020, 124, 43, 23479–23489*