Sebastian Schwan

Computational Chemist

10 December 1994

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About me

As a computational chemist and material scientist, I focus on the modelling and investigation of materials with various quantum-chemical, semiempirical and forcefield-based methods, as well as automated screening methods, machine learning and deep learning. The switch from chemistry to material science allowed me to develop a deeper understanding of physical and mathematical concepts and marks a start for my passion for programming.

Skill

Python

C, C++, Java

Shell scripting

Quantum chemical software

HPC Usage

git⋆4 sphinx⋆5 Linux⋆4 Office⋆4 Latex⋆5 Blender⋆2

(*)[The skill scale is from 0 (Fundamental Awareness) to 6 (Expert).]

INTERESTS

My professional interest focus on the investigation and development of organic and inorganic materials by utilizing various different calulation and simulation methods. By developing fully automated high-throughput screening methods and usage of machine learning for analysis, I am able to gain detailed insight into properties and structure-property relations very efficiently and quickly.

EDUCATION

2019 - 2022 Ph.D. Computational chemistry — Justus-Liebig University Giessen
Research topic: *Structuremodelling of molecular clustermaterials on different length scales*
Member of the DFG-research group FOR 2824 *Amorphous molecular materials with extremely nonlinear optical properties*

2017 - 2019 M.Sc. Material science (1.4) — Justus-Liebig University Giessen
Thesis: Modelling and investigation of co-intercalation of sodium-complexes in graphite

2014 - 2017 B.Sc. Chemistry (2.4) — Justus-Liebig University Giessen
Thesis: Investigation of adsorption of alkalimetal ions and -complexes on graphene

EXPERIENCE

2019 - 2022 Ph.D. — Physical chemical Institute, Justus-Liebig University Giessen
Thorough investigation of molecular cluster materials, structured and organized programming, use of HPC systems for materials research

2019 Study abroad in New Zealand — University of Auckland
Study at the group of Prof. Nicola Gaston (Theoretical condensed matter physics) for the investigation of small metal clusters in perovskite structures

2017 - 2019 Student assistent — Justus-Liebig University Giessen
Investigation of organic redox-active materials and development of systematic screening approach

OTHER INFORMATION

Languages

German	Native speaker
English	Fluent
Latin	School education, unpracticed since

Volunteering

2014 Pet care assistant
Animal shelter Elisabethenhof, Dorn-Assenheim

Hobbies

Technology	Computer- and home electronics, (microcontroller-) programming
Sport	Climbing and bouldering, running, hiking, biking, yoga
Music	Playing guitar, modern fingerstyle
Aquaristic	Caring for and breeding neocaridina dwarf shrimp

SKILLS AND TALENTS

Reliability	Willingness to learn	Teamplayer
Motivation	Efficiency	Adaptability
Thoroughness	Motivation	Enthusiasm

Further information and publication list: chemistschwan.github.io/