Universität Basel

Swiss Nanoscience Institute

SNI SWISS NANOSCIENCE INSTITUTE
EINE INITIATIVE DER UNIVERSITÄT BASEL UND DES KANTONS AARGAU

Development and application of new machine learning models for the quantitative prediction of biomolecular interactions.
Predictions will be validated and assessed using experimental data

Principle investigators: Prof. Anatole von Lilienfeld (Department of Chemistry, University of Basel), Prof. Michael Nash (Department of Chemistry, University of Basel)

Research
Chemical compound space is huge and has hardly been explored. Yet it might well hold the key to contribute substantially to our understanding of chemistry as well as to practical solutions for many of modern society's most pressing problems, including energy, water, planetary chemistry, or aging and disease. We develop, implement and apply the computational tools which enable us to investigate, explore, and navigate this space with physics based rigor and to unprecedented extent. For this, we rely on the principles of physical chemistry (as encoded in popular atomistic simulation codes which apply quantum mechanics, thermodynamics, and statistical mechanics to real materials), Machine Learning, and high-performance computing. We have ongoing collaborations with leading Machine Learning (incl. Google Accelerated Science) and quantum chemistry experts. The overall theme of the lab is to develop, implement and apply predictive methods which accelerate the computational design or discovery of new materials, molecules, or biomolecules using quantum mechanics (mostly DFT), Big Data, statistical mechanics, quantitative experimentation, and computing.

Details
We have recently been awarded a Swiss Nano Institute PhD scholarship, and are now looking to hire an ambitious, driven, skilled and talented individual (aka nerd) who would like to join our efforts. This PhD position is part of the SNI's PhD program which provides funding, networking opportunities, and helpful guidelines (https://nanoscience.ch/en/research/phd-program/).

Necessary skills and characteristics
-Very strong interest in chemical compound space
-Quantum chemistry knowledge
-Interest in protein sequence-structure-function relationships

-Some experience with first principles based atomistic simulation methods applied to molecules, solids or liquids (post-Hartree Fock electron correlation methods/density functional theory/semi-empirical methods) and/or stat mech methods (molecular dynamics, Monte Carlo-Programming skills and linux user experience
-For PhD position: Master of Science in physical chemistry (materials, computer science, or physics will be considered too) from an accredited institution.
-Demonstrated writing skills

Desirable experience
-Development of quantum or stat mech codes

Offer
- join our vibrant, interdisciplinary, and international research group in Basel
- collaborate with experimentalists and industrial partners
- experience a stimulating working environment: We are a member of the Institute of Physical Chemistry and the National Center for Computational Design and Discovery of Novel Materials (MARVEL), and the Swiss Nano Institute. The Biozentrum (center for molecular life sciences) is across the street, and the Swiss Nanoscience Institute is in our building. We frequently interact with other local theory groups including the ones of Goedecker and Meuwly.
- yearly renewable contracts and top salary
- Basel is a city university (oldest university in Switzerland) with international flair (bordering France and Germany) and a strong ex-pat community, not only due to university but also due to Swiss Tropical Institute, Bank for International Affairs, big pharma companies, and arts community.
- Basel is very well connected with its own airport, and high-speed trains to Paris or Frankfurt.