Sebastian Dick | CV

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EDUCATION

Stony Brook University — **Stony Brook, NY**
Ph.D. student, Physics — *2016–May 2021*

Stony Brook University — **Stony Brook, NY**
M.A., Physics — *2014–2015*

University of Wurzburg, Germany — **Wurzburg, Germany**
B.Sc. with distinction, Physics — *2011–2014*

RESEARCH

Stony Brook University — **Stony Brook, NY**
Research Assistant, Advisor: Dr. Marivi Fernandez-Serra — *May 2017–present*

- Machine learning and Density Functional Theory: Investigate how both can work together to achieve faster and more accurate electronic-structure calculations.
- NeuralXC: Developed a user-friendly Python framework to train and utilize deep learning models for electronic structure calculations
- dpyscf: Augmented existing simulation software PySCF with differentiable programming to produce scientific insights.
- libnxc: Implemented a light-weight and fast interface written entirely in C/C++ that enables the seamless integration of neural network based functionals in 30+ legacy codes.
- Co-supervised Master's students in implementing image recognition algorithms to detect defects in solids.

University of Wurzburg — **Wurzburg, Germany**
Independent research under Dr. Ronny Thomale — *Aug. 2015–Aug. 2016*

- Studied symmetry protected topological phases and conformal field theory
- Developed a C++ code ed_ising that allows for the exact diagonalization of 1-d quantum Hamiltonians under various symmetries and boundary conditions

Stony Brook University — **Stony Brook, NY**
Master thesis research, Advisor: Dr. Lukasz Fidkowski — *Jan.–July 2015*

- Analyzed short-range entangled topological phases protected by time-reversal symmetry
- Proved that the microscopic model for these phases proposed by Chen et al. and the non-linear sigma model effective field theory are equivalent.

University of Wurzburg — **Wurzburg, Germany**
Bachelor thesis research, Advisor: Dr. Ronny Thomale — *Jan.–July 2014*

- Worked with a group-internal Fortran code called FRG that uses the Functional Renormalization Group approach to study phase transitions in strongly correlated systems
- Studied the dependence of high temperature superconductivity in cuprates on doping.

PROFESSIONAL DEVELOPMENT

MLSS 2019 — **London, UK**
Machine Learning Summer School at University College London — *July 2019*

Parallel Computing in Molecular Sciences — **Berkeley, CA**
MolSSI Summer School and Workshop — *Aug. 2018*

Software Carpentry — **Stony Brook, NY**
Instructor training program — *Jan. 2018*

Became a certified Software Carpentry Instructor

TEACHING EXPERIENCE

Stony Brook University **Stony Brook, NY**
Teaching Assistant *Aug. 2016–May 2017*
Taught life science and physics students in the lab sections of introductory physics courses and graded their activities

University of Wurzburg **Wurzburg, Germany**
Teaching Assistant *Oct.–July 2016*
Taught recitation for a course on mathematical methods for physicists. Supported and graded students in the theoretical condensed matter physics graduate seminar.

PRESENTATIONS

Molecular Simulation with Machine Learning **Princeton, NJ**
Presentation *July 2020*
Title: Machine learned XC potentials in SIESTA: NeuralXC

Joint Science Meeting **Tokyo Institute of Technology, Japan**
Presentation *May 2019*
Title: Machine learning a highly accurate exchange and correlation functional of the electronic density

APS March Meeting **Boston, MA**
Presentation *Mar. 2019*
Title: Learning from the Density to Correct Total Energy and Forces in First Principle Simulations

Gordon Research Conference on Water and Aqueous Solutions **Holderness, NH**
Poster presentation *July 2018*
Presented poster: Combining DFT and Machine Learning: towards faster and more accurate ab-initio calculations of water

EXTRA-CURRICULAR ACTIVITIES

Towards Data Science
Contributing Author *Sept. 2020 - present*

IACS Professional Development Program **Stony Brook, NY**
Instructor *Sept. 2020 & Feb. 2021*

IACS Python Workshop **Stony Brook, NY**
Instructor *Jan. 2020*

IACS Diversity & Recruitment Committee **Stony Brook, NY**
Student Member *Sept. 2018–present*

Predicting Molecular Properties
Kaggle competition *Aug. 2019*
Was ranked among top 2% of all submissions

Initiative Junge Forscherinnen und Forscher e.V. **Wurzburg, Germany**
Teacher *Jan.–July 2016*
Non profit organization dedicated to teaching high school students physics and nano-science with modern classroom experiments

University of Wurzburg **Wurzburg, Germany**
Physics Student Council Member *Feb. 2012–July 2014*
Supporting and counseling physics students. Representing students' interests towards university administration.

AWARDS

"Investment" Software Fellowship **Blacksburg, VA**
MolSSI *Jan. 2020-June 2021*

Jr. Researcher Award — **Stony Brook, NY**
Institute for Advanced Computational Science — *Sep 2019*

"Seed" Software Fellowship — **Blacksburg, VA**
MolSSI — *Jan.-June 2019*

Jr. Researcher Award — **Stony Brook, NY**
Institute for Advanced Computational Science — *Sept. 2018*

DAAD Stipend
USA Exchange Program — *Sept. 2014*

LANGUAGES

German (native), English (fluent verbal and written), Italian and French (basic verbal and written)

SKILLS

Python • Fortran • C++ • OpenMP • MPI • Supervised Learning • Unsupervised Learning • Random Forest • Tensorflow • Pytorch • SQL • Bash • Git • AWS • Docker • Dashboards • Recommender Systems • Apache Spark • Sentiment Analysis

PUBLICATIONS

Sebastian Dick and Marivi Fernandez-Serra. Machine learning accurate exchange and correlation functionals of the electronic density. *Nature communications*, 11(1):1–10, 2020.

Sebastian Dick and Marivi Fernandez-Serra. Learning from the density to correct total energy and forces in first principle simulations. *The Journal of Chemical Physics*, 151(14):144102, 2019.

WRITING

Sebastian Dick. How Bayes' theorem helped win the second world war. *Towards Data Science, Editor's pick, 2020*

Sebastian Dick. Supercharge your model performance with inductive bias. *Towards Data Science, Editor's pick, 2020*

Sebastian Dick. Abstract base classes and how to use them in your data science project. *Towards Data Science, 2020*

Sebastian Dick. Unwrapping the Swiss Roll with Diffusion Maps. *Towards Data Science, Editor's pick, 2020*

SELECT PROJECTS

- **libnxc**
  Libnxc is a libary to use machine learned exchange-correlation functionals for density functional theory. All common functional types (LDA, GGA, metaGGA) as well as NeuralXC type functionals are supported. The library is written in C++ and has Fortran bindings. An implementation in Python, pylibnxc is also available. Libnxc is inspired by Libxc, mirroring as closely as possible its API. In doing so, the integration of Libnxc in electronic structure codes that use Libxc is straightforward. Libnxc can utilize multi-processing through MPI. Model inference on GPUs through CUDA is supported as well. *Skills: software development, C++*

- **neuralxc**
  Software package described in our paper "Machine learning accurate exchange and correlation functionals of the electronic density". Uses TensorFlow to implement deep neural networks that are

invariant with respect to atom permutation and global rotations. The neural network is used to parametrize a functional that maps the electron density of a given system–a 3-d scalar field–to its energy. Applications to modelling properties of molecules and solids at the quantum mechanical level.
Skills: deep learning, software development, TensorFlow, PyTorch

- **twitter-sentiment-tracker**
  Plotly based web-abb to discover cultural and market trends by tracking sentiments towards key topics expressed on twitter. The app uses Twitter's filtered search API along with the textblob python library to extract tweets and analyze users' sentiments. Data stream is handled by AWS Kinesis and sentiment extraction at scale is achieved using Spark.
  Skills: AWS, Apache Spark, Databricks, ETL, streaming data, sentiment analysis, dash/plotly

- **paper-scraper**
  A tool to interactively explore research articles posted on the arXiv. It taylors recommendations by inferring users' interests from their bookmarked articles. Starting from these recommendations users can explore related research by traversing a connected network of articles.
  Skills: AWS, Docker, dash/plotly, spectral-clustering, recommender systems, gensim

- **tensorfield-torch**
  PyTorch implementation of "tensor field networks" (Thomas et al.). Uses tensor products between irreducible representations of symmetry groups to define equivariant neural network layers. Extends original functionality by adding on-site tensor interactions.
  Skills: deep learning, PyTorch, group theory