Sebastian Dick | CV

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EDUCATION

Stony Brook University Stony Brook, NY Ph.D. student, Physics

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

University of Wurzburg, Germany

B.Sc. with distinction, Physics 2011-2014

RESEARCH

Stony Brook University

Stony Brook, NY

Wurzburg, Germany

2016-present

Research Assistant, Advisor: Dr. Marivi Fernandez-Serra

May 2017-present

- o Machine learning and Density Functional Theory: Investigate how both can work together to achieve faster and more accurate electronic-structure calculations.
- o NeuralXC: Development of a Python framework that lets users train and use density functionals based on machine
- o Physics inspired deep learning: Encode physical symmetries in neural network architectures to improve generalization. Work on equivariant neural networks.

University of Wurzburg

Wurzburg, Germany

Independent research under Dr. Ronny Thomale

Aug. 2015-Aug. 2016

- o 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

- o Analyzed short-range entangled topological phases protected by time-reversal symmetry
- o 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

July 2019

Jan. 2018

- o 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

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

Software Carpentry Stony Brook, NY

Instructor training program

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

IACS Diversity & Recruitment Committee

Stony Brook, NY

Student Member

experiments

Sept. 2018–present

Initiative Junge Forscherinnen und Forscher e.V.

Wurzburg, Germany

Jan.–*July* 2016 Non profit organization dedicated to teaching high school students physics and nano-science with modern classroom

University of Wurzburg

Physics Student Council Member

Wurzburg, Germany 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, Tensorflow, Pytorch, MySQL, Bash, Git

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.