Artem Pulkin

[er'ts'əm]

Postdoctoral researcher at QuTech TU Delft

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🔍 jobs: **researcher, research engineer, data scientist, software engineer**

Currently

Developing innovative machine learning approaches to engineer electronic materials and molecules addressing modern society challenges

Expertise

Computational condensed matter, quantum chemistry, numerical materials science, machine learning, many-body physics, research code development.

Education 🎓

Docteur ès Sciences EPFL in physics Lausanne CH 🇨🇭 Specialized on: numerical electronic structure, quantum simulations. Thesis: Electronic Transport in 2D Materials with Strong Spin-orbit Coupling (03/2017); supervisor: Oleg Yazyev	2012-2017
Master of Science Chalmers in applied physics Göteborg SE 🇸🇪 Thesis: Spintromechanical Aspects of Charge Transport in Nanostructures (06/2012); supervisor: Robert Shekhter	2010-2012
B.Sc. in Physics cum laude V.N. Karazin's State University Kharkiv UA 🇺🇦	2006-2010

Research 🔬

Postdoc @ QuTech and Kavli Institute of Nanoscience, Delft university of technology NL 🇳🇱	2019-now
Researching a stack of machine learning tools: deep neural networks DNN, generative models (reverse Monte-Carlo, RMC), adversarial attack approaches in the context of electronic structure/nanoscale atomic dynamics. Developing a DNN/atomic descriptor code for nanoscale dynamics miniff. Discovering novel electronic materials as a part of a multi-disciplinary team of quantum researchers.	
Postdoc @ Caltech US 🇺🇸	Jul'17-Mar'19
Developed and implemented a computational many-body quantum chemistry framework to model two-dimensional crystalline materials. Investigated low-energy spectral properties of two-dimensional molybdenum disulphide with numerical modeling.	
Doctoral assistant @ EPFL CH 🇨🇭	Oct'12-Apr'17
Carried out a scientific project in the quantum materials modelling domain. Discovered a new class of electronic band structure effects in two-dimensional semiconductors. Collaborated with world-leading experimental groups to prove my findings experimentally.	
Research assistant @ Seoul National University, KR 🇰🇷	Jun'12-Aug'12
Research assistant @ Chalmers, SE 🇸🇪	Aug'10-Jun'12

In numbers

15 publications **>500** citations **14** talks

>10 countries

>30 collaborators

Software

More on github/pulkin.

miniFF https://gitlab.kwant-project.org/qt/miniff (python, cython)

Simulate molecular dynamics with classical force fields and machine learning. Combines the power of cython, numpy and torch to deliver maximal performance in a high-quality python code.

miniFF

pyscf https://github.com/pyscf/pyscf (python, C)

A large collaboration across universities and public companies towards high-performance Quantum chemistry in python. I contributed towards implementing periodic boundary conditions for diagrammatic kernels.

pyteleport https://github.com/pulkin/pyteleport

Pause, teleport and resume your python runtime from within the stack. Manipulates cPython memory and bytecode.

dfttools https://github.com/pulkin/dfttools (python)

Parsing and plotting the results of first-principles simulations.

openmx-hks https://github.com/pulkin/openmx-hks (C)

A practical tool to convert the data from a popular density functional theory code into numpy.

micropython https://github.com/pulkin/micropython (C)

A micropython port to a popular cellular network module A9G.

Awards 🏆

💰 Personal **Swiss NSF grant** to study abroad 80k CHF, 18 months, postdoctoral level (Early Postdoc.Mobility) grant P2ELP2_175281   **postgraduate**

💰 Personal computing time at **national supercomputing facilities (SURF NL)** Approximate equivalent of 26k EUR, 24 months project 45873

🥇 Olympiad in Physics for University Students (national in Ukraine) – **first prize**   **graduate**

🥇 **Youth Physicists Tournament** (national in Ukraine, team) – multiple prizes

🥇 Open Olympiad in Applied Physics (MIPT Moscow) – **first prize**

💰 Kharkiv City Mayor and Kharkiv State Governor scholarships for gifted youth

🥇 Dozens of prizes in physics and informatics (olympiads, student projects; **top-10 and top-1 in national competitions**)   **high school**

💰 Multiple scholarships

Skills 🔨

Science: quantum condensed matter, first-principles approaches.

Machine learning: supervised learning, deep neural networks (DNN), dataset generation, feature extraction, generative modelling, adversarial attacks.

Software development in 🐍 Python (6 years): numpy, torch, matplotlib; notebooks; HPC and parallel/distributed/concurrent computing (MPI, OpenMP, multiprocessing); performance-driven development with C and cython; styling, testing, documenting, packaging; micropython and python beyond standards (cPython bytecode).

C: HPC and parallel environments (MPI, OpenMP); Lapack; embedded platforms.

Other: ☕ Java, Fortran, Julia, Javascript, Matlab.

Infrastructure: git, CI/CD (Travis, Gitlab-CI, Azure pipelines).

IDEs: Pycharm, vim.

Soft skills: critical analysis, problem solving, communicating (organizing discussions, presenting, paper/grant/documentation writing), full-cycle project management (idea - funding - implementation - reporting), supervision.

Languages

English (proficient), Russian (mother), French (basic), Dutch (basic).

Hobbies

Sports, ✈ travels, cross-stitching, soldering, 🔒 lock picking, 🕹 board and video games, open-source projects.