

# Artem Pulkin

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Postdoctoral researcher at QuTech TU Delft

✉ gpulkin@gmail.com 🌐 pulk.in 🏠 Amsterdam NL 🇳🇱

🔍 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 quantum, machine learning, 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](https://github.com/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.



**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, postgraduate postdoctoral level (Early Postdoc.Mobility) grant P2ELP2\_175281

💰 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.