Artem Pulkin

[ɐrˈtsʲɵm]

Postdoctoral researcher at QuTech TU Delft

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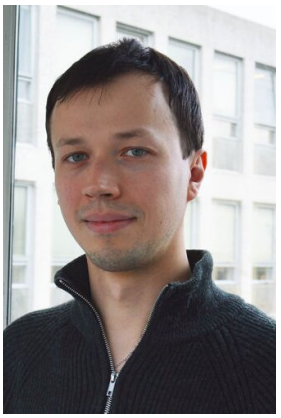
jobs: **researcher, research engineer, data scientist, software engineer**



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 Delft university of technology NL — Apr 2019-now

I am developing novel approaches based on machine learning to predict molecular dynamics and electronic structure properties of amorphous topological insulator materials. I am supervising a multi-disciplinary team of condensed matter and quantum nanoscience researchers aiming for real-world applications of these materials.

Postdoc @ Caltech US — Jul'17-Mar'19

I successfully carried out an ambitious postdoctoral project funded by a personal Swiss NSF grant P2ELP2_175281 in collaboration with prof. Garnet Chan group from Caltech. I developed and implemented first of its kind computational many-body quantum chemistry framework to model two-dimensional crystalline materials. I demonstrated the power of the approach by computing low-energy spectral properties of two-dimensional molybdenum disulphide.

Doctoral assistant @ EPFL CH — Oct'12-Apr'17

I discovered a new class of electronic band structure effects in two-dimensional transition metal dichalcogenides originating from the interplay of spin-orbit interactions and crystalline lattice symmetries. In collaboration with world-leading experimental groups, I was able to demonstrate these effects in real materials resulting in several high-impact publications.

Research assistant @ Seoul National University, KR — Jun'12-Aug'12

I studied electronic structure of edge states in models of overlapping topological graphene nanoribbons.

Research assistant @ Chalmers, SE — Aug'10-Jun'12

I designed a concept of a nanoscale spin-mechanical single-electron transistor (SET).

Teaching

Presenter at a mini-course on Electronic structure methods in TUD — 2020-now

Teaching assistant at Computational physics III EPFL: conducting practice sessions, guiding B.Sc. and M.Sc. students, preparing examination, grading — 2013-2016

Teaching assistant at General physics EPFL: conducting practice sessions, answering students' questions — Fall 2015

Teaching assistant at Analysis III EPFL: conducting practice sessions, answering students' questions, preparing examination problems — Fall 2014

Teaching assistant at Physics Workshop EPFL: conducting lab work in small groups of students, grading — Fall 2013

Teacher of physics at Kharkiv high school 45: guiding high school students through advanced physics problem solving, preparing to physics competitions — 2007-2010

Funding 💰

Computing time at national supercomputing facilities (SURF NL) Approximate equivalent of 26k EUR, 24 months project 45873 — 2020-now

Personal Swiss NSF grant to study abroad 80k CHF, 18 months, postdoctoral level (Early Postdoc.Mobility) grant P2ELP2_175281 — 2017-2019

Supervision

Katya Fouka, Masters @ Leiden University — 2021

Extracurricular

Organizing a course on numerical modelling techniques with a focus on first-principles problems — 2019-now

Co-organized a tensor network journal club with a focus on mathematical aspects of tensor network computations — 2018

Participated as a jury member in International Physics Tournament held in Lausanne CH — 2013

Skills 🔨

Theory: quantum condensed matter; first-principles approaches: Hartree-Fock, density functional theory (DFT), quantum chemistry (diagrammatic approaches); classical thermodynamics; machine learning.

Numerics and simulations: second quantization, tight-binding, neural and tensor networks, classical force fields, large-scale simulations, high-performance computing.

Codes, languages, packages: python (numpy, keras, pytorch, matplotlib, cython, core development: cPython, uPython), C, Java, Matlab, bash; Quantum Espresso, OpenMX, pyscf.

Soft: 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).

Publications

📄 **Artem Pulkin**, Daniel Varjas — in preparation

Topological electronic properties of amorphous Bi2Se3

📄 **Artem Pulkin**

A neural-network classical potential for simulating disorder in amorphous Bi2Se3

📄 **Artem Pulkin**, Niket Agrawal, André Melo — 2021

miniff – A minimal implementation of classical and neural-network force fields in python

Zenodo doi:10.5281/zenodo.4626641 (2021) 🔗 link code

📄 **Artem Pulkin**, Oleg Yazyev — 2020

Controlling the Quantum Spin Hall Edge States in Two-Dimensional Transition Metal Dichalcogenides

J. Phys. Chem. 11, issue 17 p. 6964 (2020) 🔗 arXiv

📄 PySCF team

Recent developments in the PySCF program package

J. Chem. Phys. 153, 024109 (2020) 🔗 arXiv

📄 **Artem Pulkin**, Garnet Kin-Lic Chan

First principles coupled cluster theory of the electronic spectrum of the transition metal dichalcogenides

Phys. Rev. B 101 241113(R) (2020) arXiv

Zahra Pedramrazi, Charlotte Herbig, **Artem Pulkin**, Shujie Tang, Madeleine Phillips, Dillon Wong, Hyejin Ryu, Michele Pizzochero, Yi Chen, Feng Wang, Eugene J Mele, Zhi-Xun Shen, Sung-Kwan Mo, Oleg V Yazyev, Michael F Crommie — 2019

Manipulating Topological Domain Boundaries in the Single-Layer Quantum Spin Hall Insulator 1T′–WSe2

Nano lett. 19 (8) 5634-5639 (2019) ACS

Sara Barja, Sivan Refaely-Abramson, Bruno Schuler, Diana Y. Qiu, **Artem Pulkin**, Sebastian Wickenburg, Hyejin Ryu, Miguel M. Ugeda, Christoph Kastl, Christopher Chen, Choongyu Hwang, Adam Schwartzberg, Shaul Aloni, Sung-Kwan Mo, D. Frank Ogletree, Michael F. Crommie, Steven G. Louie, Jeffrey B. Neaton, Oleg V Yazyev, and Alexander Weber-Bargioni

Identifying substitutional oxygen as a prolific point defect in monolayer transition metal dichalcogenides

Nat. comm. 10 (1), 3382 (2019) arXiv

Miguel M. Ugeda, **Artem Pulkin**, Shujie Tang, Hyejin Ryu, Quansheng Wu, Yi Zhang, Dillon Wong, Zahra Pedramrazi, Ana Martín-Recio, Yi Chen, Feng Wang, Zhi-Xun Shen, Sung-Kwan Mo, Oleg V. Yazyev and Michael F. Crommie — 2018

Observation of Topologically Protected States at Crystalline Phase Boundaries in Single-layer WSe2

Nat. Commun. 9 3401 (2018) arXiv

Artem Pulkin, and Oleg V. Yazyev — earlier

Robustness of the quantum spin Hall insulator phase in monolayer 1T’ transition metal dichalcogenides

J. Electron Spectrosc. Relat. Phenom. 219 72-76 (2017) ScienceDirect

Artem Pulkin, and Oleg V. Yazyev

Spin- and valley-polarized transport across line defects in monolayer MoS2

Phys. Rev. B 93 041419 (2016) arXiv

Ossi Lehtinen, Hannu-Pekka Komsa, **Artem Pulkin**, Michael Brian Whitwick, Ming-Wei Chen, Tibor Lehnert, Michael J. Mohn, Oleg V. Yazyev, Andras Kis, Ute Kaiser, and Arkady V. Krasheninnikov

Atomic scale microstructure and properties of Se-deficient two-dimensional MoSe2

ACS Nano 9 (3) 3274–3283 (2015) ACS

T. Eelbo, M. Waśniowska, M. Sikora, M. Dobrzański, A. Kozłowski, **A. Pulkin**, G. Autès, I. Miotkowski, O. V. Yazyev, and R. Wiesendanger

Strong out-of-plane magnetic anisotropy of Fe adatoms on Bi2Te3

Phys. Rev. B 89 104424 (2014) arXiv

Robert I. Shekhter, **Artem Pulkin**, Mats Jonson

Spintronic mechanics of a magnetic nanoshuttle

Phys. Rev. B 86, 100404(R) (2012) APS

Anatoli M. Kadigrobov, Robert I. Shekhter, Igor Aronov, Sergeij I. Kulinich, **Artem Pulkin**, Mats Jonson

Microwave-induced spin-flip scattering of electrons in point contacts

Low Temperature Physics/Fizika Nizkikh Temperatur, 37 (11) 925 AIP

*links online

Presentations

Electronic properties of amorphous topological insulator from first principles Real-space Simulations of Topological Matter and Disordered Materials (IOP) **UK** — 2021

Neural network approach to the amorphous topological insulator Bi2Se3 Physics@Veldhoven 2021 **NL**

Coupled-cluster study of two-dimensional transition metal dichalcogenides, Physics@Veldhoven 2020 **NL** — 2020

📢 Electronic and spin transport properties of two-dimensional transition metal dichalcogenides, WE-Heraeus-Seminar / Spin Transport in Complex Magnetic Structures, Bad Honnef **DE** 🇩🇪

📢 First-principles coupled-cluster study of two-dimensional materials, Thomas Young Center Lunchtime Seminar Series, Imperial College, London **UK** 🇬🇧 2019

📢 Micropython on GSM microcontroller, Python meetup Rotterdam 2019, Rotterdam **NL** 🇳🇱

📢 First-principles diagrammatic methods, Entanglement in Strongly Correlated Systems school, Benasque **ES** 🇪🇸

📢 First-principles diagrammatic simulations of two-dimensional crystals, Uni Leiden **NL** 🇳🇱

📢 First-principles diagrammatic simulations of solids, Uni Amsterdam **NL** 🇳🇱

📢 Electronic Properties of Materials Using Coupled-cluster Approach, Vrije Universiteit Amsterdam **NL** 🇳🇱

📢 Electronic Transport and Topological Properties of 2D Transition Metal Dichalcogenides, Uni Delft **NL** 🇳🇱

📢 The density matrix embedding theory, Technical University of **Denmark** 🇩🇰 2018

📢 2D Materials with Strong Spin-orbit Coupling: Topological and Electronic Transport Properties, Novel Quantum States in Condensed Matter conference, Kyoto **JP** 🇯🇵 earlier

📢 Electronic structure of line defects in 2D transition metal dichalcogenides: a transport perspective, SPS Annual Meeting, Lugano **CH** 🇨🇭

📢 Spin- and Valley-Polarized Transport across Line Defects in Monolayer MoS2, APS March Meeting, Baltimore **US** 🇺🇸

Hobbies

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