

Artem Pulkin

[er'tsiəm]

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🏠 Amsterdam NL 🇳🇱

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

Training

Coursera: Machine Learning from Stanford University

Research 🧪

Postdoc @ QuTech Delft university of technology NL 🇳🇱 Apr '19-Apr '22

I developed novel approaches based on machine learning to predict molecular dynamics and electronic structure properties of amorphous topological insulator materials. I supervised a multi-disciplinary team of condensed matter and quantum nanoscience researchers working on 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 (prof), Ukrainian (mother), Russian, 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 ACS


 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.