

# Artem Pulkin

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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 physics, 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).

## 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, pycsf.

**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 Bi<sub>2</sub>Se<sub>3</sub>

📄 **Artem Pulkin**

A neural-network classical potential for simulating disorder in amorphous Bi<sub>2</sub>Se<sub>3</sub>

📄 **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'-WSe<sub>2</sub>

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 WSe<sub>2</sub>

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 MoS<sub>2</sub>

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 MoSe<sub>2</sub>

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 Bi<sub>2</sub>Te<sub>3</sub>

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 Bi<sub>2</sub>Se<sub>3</sub> 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 MoS<sub>2</sub>, APS March Meeting, Baltimore **US** 

## Hobbies

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