Artem Pulkin

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Amsterdam NL

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

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).

Skills

Theory and numerics: quantum condensed matter, first-principles approaches (HF, DFT, coupled cluster, tensor networks, embedding), machine learning, quantum computing.

Codes, languages, packages: python (numpy, 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

Antonio L. R. Manesco, AP — 2022

Spatial separation of spin currents in transition metal dichalcogenides

arXiv

AP, 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

AP, 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

AP, 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, AP, 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, AP, 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, AP, 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

AP, 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

AP, 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, AP, 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, AP, 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, AP, 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, AP, 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

2021

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

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

2020

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

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

2019

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

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**

2018

The density matrix embedding theory, Technical University of **Denmark**

earlier

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

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.