Curriculum Vitae

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Tolibjon Abdurakhmonov

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Date of birth: July 25, 1996
Place of birth: Uzbekistan

SUMMARY OF QUALIFICATIONS

Master of Science: *Theoretical Physics*

EDUCATION & EMPLOYMENT

Jul. 2022 – now	**PhD | Research Assistant** *(Prof. O. Kühn's group, Institute of Physics, University of Rostock)*
Jan. 2022 – Jun. 2022	**Reseach Intern** *(Physical-Technical Institute, NGO "Physics-Sun")*
Dec. 2020 – Jun. 2022	**Teaching Assistant** (part time) *(INHA University in Tashkent)*
Sep. 2020 – Jan. 2022	**Junior Researcher** *(UT-FA-2020-3 grant, Institute of Nuclear Physics of Uzbekistan Academy of Sciences)*
Sep. 2019 – May. 2021	**Master Student** *(Department of Physics, National University of Uzbekistan)*
Sep. 2015 – Jun. 2019	**Bachelor Student** *(Department of Physics, National University of Uzbekistan)*

RESEARCH INTERESTS

Electronic Structure Methods, Molecular Mechanics, Force Field parametrization, Computational Material Science, E(3) Graph Neural Networks for excited states, Exciton Dynamics

RELEVANT EXPERIENCES

Force Field & parametrization
Density Functional Theory (DFT)
Extended Tight-Binding method (xTB)
Kinetic Monte Carlo
Teaching:
- Form Molecules to Solids – seminar since 2023;
- Machine Learning Interatomic Potentials (research lab course)
Experience in HPC management (since 04.2025)

Frenkel-Holstein model for aggregates
Molecular Dynamics simulations
Molecular aggregates on substrates
Self-assembly of molecules on 2D interfaces

SKILLS

Computational skills:	Python, Bash, Gaussian, VASP, LAMMPS, DFTB+, PySCF, ASE, PyTorch, Excipy
Operating systems:	Linux, MacOS, Qlustar
Computer Literacy:	IT & System Administration, Server & Cluster Management, HPC support
Languages:	English, Russian, Uzbek

PUBLICATIONS

1. C. Rehhagen, T. Abdurakhmonov, M. Frank, O. Kühn[1], S. Lochbrunner - Exciton Interaction and Diffusion in Perylene Derivative Microcrystals (2025) (in preparation)

2. T. Abdurakhmonov and O. Kühn - Interlayer Force Field for the Anisotropic Interaction between Planar Organic Molecules and Two-dimensional Hexagonal Boron Nitride, ACS JCTC (2025) DOI: 10.26434/chemrxiv-2025-kvl69
3.
4. N. le Coutre, T. Abdurakhmonov, P. Weinbrenner, K. Watanabe, T. Taniguchi, T. Korn, F. Fennel, O. Kühn and F. Reinhard - Growth of Few-Layer Molecular Crystals of PTCDI on Hexagonal Boron Nitride by Microspacing Air-Gap Sublimation, ACS Applied Optical Materials *3* (2), 455-462 (2025). DOI: 10.1021/acsaom.4c00522

5. A.Rakhimov, T. Abdurakhmonov, Z. Narzikulov and V.I. Yukalov - Self-consistent theory of a homogeneous binary Bose mixture with strong repulsive interspecies interaction, Phys. Rev. A 106, 033301 (2022). DOI: 10.1103/PhysRevA.106.033301

6. A.Rakhimov, T. Abdurakhmonov and B. Tanatar - Critical behavior of Tan's contact for bosonic systems with a fixed chemical potential, J. Phys.: Condens. Matter 33, 465401 (2021) DOI: 10.1088/1361-648X/ac1ec6

CONFERENCE and WOKSHOPS

1. T. Abdurakhmonov and O. Kühn – *Self-assembly of PTCDI molecules on Two-dimensional Hexagonal Boron Nitride,* **International Conference LiMatI 2024**, (talk) University of Rostock, September 23-27, 2024. Rostock, Germany.

2. T. Abdurakhmonov and O. Kühn – *Interlayer Potential parametrization for planar dye molecules on Hexagonal Boron Nitride*, (poster) **CCP5 Summer School 2024,** July 14-25, 2024. Newcastle upon Tyne, UK.

3. **IRTG Summer School 2024**, May 21-23, 2024. University of Rostock. Rostock, Germany.

4. T. Abdurakhmonov and O. Kühn – *Molecular Dynamics insight into Adsorption properties: Interlayer Potential parametrization for dye molecules on Hexagonal Boron Nitride layers*, (poster) "**Machine Learning for Chemistry" workshop,** February 27 – March 1, 2024. Bad Hofgastein, Austria.

5. T. Abdurakhmonov and O. Kühn – *Adsorption properties of organic dye molecules on Hexagonal Boron Nitride layers*, (poster) "**Wavefunction Methods for Solid State Matter" training workshop,** December 5-8, 2023. Gdynia, Poland.

6. T. Abdurakhmonov **- LiMatI Summer School 2022**, September 12-14, 2022. Institute of Physics, University of Rostock. Rostock, Germany.

7. A. Khudoyberdiyev, A. Rakhimov and T. Abdurakhmonov – *Restriction on the phase angle of the triplon gas wave function,* **7st ICSM** November 21-28, 2021. Bodrum, Turkey.

8. T. Abdurakhmonov and A. Khudoyberdiyev – *Tan's contact of quantum magnets at finite temperature,* (talk) **1st Republican Conference of Young Scientists and Students**. April 14-15, 2021. Tashkent, Uzbekistan.