

Almaz Khabibrakhmanov

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Personal webpage
ORCID
Google Scholar
LinkedIn

ABOUT MY WORK

I develop first-principles methods that unify quantum mechanical descriptions of van der Waals dispersion with machine-learned force fields, enabling accurate, scalable simulations of condensed matter that were previously out of reach. To date, I have published nine peer-reviewed articles, see the full publication list at the end.

FIELDS OF EXPERTISE

- van der Waals Interactions
- Density Functional Theory
- Interatomic Potentials
- Chemical Physics
- Materials Science

EDUCATION

01/2021 – 03/2025 **Ph.D. in Physics, University of Luxembourg**
Thesis: *"Bridging quantum Drude oscillators and electronic-structure theory for van der Waals dispersion interactions"*
Advisor: Prof. Alexandre Tkatchenko (Theoretical Chemical Physics Group)

09/2018 – 08/2020 **M.Sc. in Applied Mathematics and Physics, Moscow Institute of Physics and Technology**
Major: Solid State Physics & Materials Science, GPA: 9.7/10
Thesis: *"Theoretical study of diamond-like carbon nanostructures and their stiffness"*
Advisor: Prof. Pavel Sorokin (Laboratory of Novel Materials Modeling)

09/2014 – 08/2018 **B.Sc. in Applied Mathematics and Physics, Moscow Institute of Physics and Technology**
Major: Molecular & Chemical Physics, GPA: 9.5/10
Thesis: *"Theoretical investigation of the atomic structure and mechanical properties of novel dense sp^3-carbon nanostructures"*
Advisor: Prof. Pavel Sorokin (Laboratory of Novel Materials Modeling)

PROFESSIONAL EXPERIENCE

03/2025 – 01/2026 **Postdoctoral Researcher, University of Luxembourg**
Developed reduced-density matrix formulation of many-body dispersion; co-developed a framework for modeling covalent bonding using quantum Drude oscillators (QDO); co-developed MBD-ML model (manuscripts submitted/in preparation)
Advisor: Prof. Alexandre Tkatchenko (Theoretical Chemical Physics Group)

03/2022 – 06/2022 **Visiting Graduate Researcher, University of California, Los Angeles**
Institute for Pure and Applied Mathematics (IPAM), core participant
Long Program *"Advancing Quantum Mechanics with Mathematics and Statistics" (QMM)*

01/2021 – 03/2025 **Doctoral Researcher, University of Luxembourg**
Developed universal pairwise vdW-QDO potentials; contributed to developing SO3LR machine-learning force-field; studied dispersion-induced density polarization effect
Advisor: Prof. Alexandre Tkatchenko (Theoretical Chemical Physics Group)

10/2017 – 12/2020 **Research Assistant, TISNCM (Moscow) and NUST "MISiS" (Moscow)**
Performed density-functional theory calculations; developed a model for stiffness of carbon nanostructures; studied electronic properties of graphene oxide
Advisor: Prof. Pavel Sorokin (Laboratory of Novel Materials Modeling)

SERVICE

2023 – present **Peer Reviewer**
Journal of Chemical Theory and Computation, The Journal of Chemical Physics
Reviewed three research articles

09/2021 – 06/2023 **Teaching Assistant, University of Luxembourg**
Computational Methods & *Quantum Mechanics* (one semester each)
Led exercise sessions; prepared teaching materials and exams; graded exams

SOFTWARE EXPERIENCE

- **Code Contributions:**
  - ✓ Implemented vdW-QDO potential in LAMMPS (C++)
  - ✓ Implemented MBD@FCO in libMBD/FHI-aims (Fortran)
  - ✓ Modified XDM routines in FHI-aims (Fortran)
- **Coding & Computing:**
  - ✓ Python (fluent: data analysis, visualization)
  - ✓ HPC (MPI/OpenMP, Slurm), Fortran, C++
- **Scientific Software:**
  - ✓ **DFT**: FHI-aims, VASP, SIESTA
  - ✓ **Quantum Chemistry**: PySCF, Q-Chem, ORCA, MRCC
  - ✓ **Molecular Dynamics**: LAMMPS, ASE
  - ✓ **Visualization**: OVITO, VESTA, ChimeraX

AWARDS & HONORS

- **Best Poster Award** at the NCAITMS conference, Warsaw (2025)
- ***Summa cum Laude*** graduation from B.Sc. (2018) and M.Sc. (2020)
- **Letter of acknowledgement**, Ministry of Science and Higher Education (2020)
- **Increased Academic Scholarship** for excellence in study (2017 – 2020)
- **Alexander Abramov Fund Scholarship** for excellence in study (2015 – 2017)

LANGUAGES

- Russian — Native
- Tatar — Native
- English — C1
- French — B1
- Luxembourgish — A2
- German — A1

CONFERENCES & WORKSHOPS

- **Invited Talks/Seminars:**
  - ✓ Reunion Meeting of the IPAM QMM Long Program, Los Angeles (2024)
  - ✓ Seminar in the groups of Prof. Giulia Galli and Prof. Laura Gagliardi, University of Chicago (2024)
  - ✓ *"The van der Waals – London Discussions"*, University of Strasbourg (2023)
- **Contributed Talks:**
  - ✓ German Physical Society (DPG) Spring Meeting, Berlin (2024)
  - ✓ *"Intermolecular Interactions and Properties of Gases, Liquids and Solids"*, Graz (2023)
  - ✓ *"Electronic Structure Theory and Machine Learning in Materials Science and Computational Chemistry"*, Levi, Finland (2023)
  - ✓ IPAM QMM 2022 Long Program, Los Angeles (2022)
  - ✓ American Physical Society (APS) March Meeting, Chicago (2022)
- **Posters:**
  - ✓ *"New Challenges for Ab Initio Theory in Molecular Science"* (NCAITMS), Warsaw (2025)
  - ✓ 13th Triennial WATOC Congress, Oslo (2025)
  - ✓ 6th Psi-k Conference, Lausanne (2022)
  - ✓ CECAM Workshop "*Non-Covalent Interactions in Large Molecules and Extended Materials*", Lausanne (2021)

PUBLICATIONS

10 peer-reviewed publications (incl. 6 as first author), >290 citations on Google Scholar, h-index = 7

† marks equal contributions

1. **MBD-ML: Many-Body Dispersion from Machine Learning for Molecules and Materials**
   E. Moerman, A. Kabylda, A. Khabibrakhmanov, A. Tkatchenko, *PRX Intelligence* **1**, 013003 (2026)
2. **Noncovalent Interactions in Density Functional Theory: All the Charge Density We Do Not See**
   A. Khabibrakhmanov, M. Gori, C. Müller, A. Tkatchenko, *J. Am. Chem. Soc.* **147**, 40763-40775 (2025)
3. **Accurate Noncovalent Interactions in Atomistic Systems via Quantum Drude Oscillators**
   A. Khabibrakhmanov, D.V. Fedorov, A. Ambrosetti, J. Crain, K.L.C. Hunt, E.R. Johnson, K.D. Jordan, S. Góger, M. Gori, M.R. Karimpour, R.J. Maurer, M. Sadhukhan, M. Stöhr, A. Tkatchenko, *J. Chem. Phys.* **163**, 151001 (2025)
4. **Molecular Simulations with a Pretrained Neural Network and Universal Pairwise Force Fields**
   A. Kabylda, J. T. Frank, S. Suárez-Dou, A. Khabibrakhmanov, L. M. Sandonas, O. T. Unke, S. Chmiela, K.-R. Müller, A. Tkatchenko, *J. Am. Chem. Soc.* **147**, 33723-33734 (2025)
5. **Universal Pairwise Interatomic van der Waals Potentials Based on Quantum Drude Oscillators**
   A. Khabibrakhmanov, D.V. Fedorov, A. Tkatchenko, *J. Chem. Theory Comput.* **19**, 7895-7907 (2023)
6. **Optimized Quantum Drude Oscillators for Atomic and Molecular Response Properties**
   S. Góger†, A. Khabibrakhmanov†, O. Vaccarelli†, D.V. Fedorov, and A. Tkatchenko, *J. Phys. Chem. Lett.* **14**, 6217-6223 (2023)
7. **Electronic Properties of Graphene Oxide: Nanoroads towards Novel Applications**
   A.I. Khabibrakhmanov, P.B. Sorokin, *Nanoscale* **14**, 4131-4144 (2022)
8. **Extended UV Detection Bandwidth: h-BN/Al Powder Nanocomposites Photodetectors Sensitive in a Middle UV Region Due to Localized Surface Plasmon Resonance Effect**
   I.N. Volkov, Z.S. Yermekova, A.I. Khabibrakhmanov, A.M. Kovalskii, S. Corthey, A.R. Tameev, A.E. Aleksandrov, P.B. Sorokin, D.V. Shtansky, and A.T. Matveev, *Europhys. Lett.* **133**, 28002 (2021)
9. **Carbon on the nanoscale: Ultrastiffness and unambiguous definition of incompressibility**
   A. Khabibrakhmanov, P. Sorokin, *Carbon* **160**, 228–235 (2020)
10. **Ultrasmall diamond nanoparticles with unusual incompressibility**
    M. Popov, V. Churkin, D. Ovsyannikov, A. Khabibrakhmanov, A. Kirichenko, E. Skryleva, Y. Parkhomenko, M. Kuznetsov, S. Nosukhin, P. Sorokin, S. Terentiev, V. Blank, *Diam. Relat. Mater.* **96**, 52–57 (2019)

DATASETS

1. **Data for "Noncovalent Interactions in Density Functional Theory: All the Charge Density We Do Not See"**
   A. Khabibrakhmanov, *Zenodo* (2026)