DR. MATEJ DITTE

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FIELDS OF INTEREST

computational quantum chemistry and material science, electronic structure and correlations, dispersion interactions, quantum Monte Carlo, density functional theory (+ vdW), embedding methods

ACADEMIC POSITIONS

University of Luxembourg *Mar. 2024 - Aug. 2024*
Position: Postdoctoral researcher
Supervisor: Prof. Alexandre Tkatchenko
Topics: dispersion interactions. quantum embedding

University of Luxembourg *Nov. 2019 - Feb. 2024*
Position: Doctoral researcher
Supervisor: Prof. Alexandre Tkatchenko
Topics: dispersion interactions. quantum embedding

University of Ostrava *Jul. 2018 - Oct. 2019*
Position: Research assistant
Supervisor: Dr. Matúš Dubecký
Topics: non-covalent interactions, fractional charge, excited states, quantum Monte Carlo

EDUCATION

University of Luxembourg *Nov. 2019 - Jan. 2024*
Doctoral Degree in Physics
Thesis: Molecules in Environments: Towards Systematic Quantum Embedding of Electrons and Drude Oscillators
Supervisor: Prof. Alexandre Tkatchenko

Comenius University in Bratislava *Sep. 2016 - Jun. 2019*
Master Degree in Solid-State Physics Overall Average: 1.08
Thesis: Protocol development for calculating excited states of molecules using Diffusion Monte Carlo
Supervisor: Dr. René Derian

Comenius University in Bratislava *Sep. 2013 - Jun. 2016*
Bachelor Degree in Physics Overall Average: 1.52
Thesis: Study of quantum correlation effects in a system of interacting fermions
Supervisor: Dr. René Derian

PUBLICATIONS

QMeCha: Quantum Monte Carlo package for fermions in embedding environments
M. Barborini, J. Charry, M. Ditte, A. Leventis, G. Kafanas, and A. Tkatchenko, J. Chem. Phys. **164**, 062501 (2026)

Chalcogen Bonding with Telluronium Cations: toward Selective Population of Tellurium σ-Holes by Lewis Bases
L. Groslambert, Y. Cornaton, P. Pale, M. Ditte, A. Tkatchenko, J.-P. Djukic, and V. Mamane, J. Org. Chem. **90**, 8254 (2025)

Molecule-Environment Embedding with Quantum Monte Carlo: Electrons Interacting with Drude Oscillators
M. Ditte, M. Barborini, and A. Tkatchenko, J. Chem. Theory Comput. **21**, 4466 (2025)

Quantum Drude Oscillators Coupled with Coulomb Potential as an Efficient Model for Bonded and Non-Covalent Interactions in Atomic Dimers
M. Ditte, M. Barborini, and A. Tkatchenko, J. Chem. Phys. **160**, 094309 (2024)

Affinity of Telluronium Chalcogen Bond Donors for Lewis Bases in Solution: A Critical Experimental-Theoretical Joint Study
L. Groslambert, Y. Cornaton, M. Ditte, E. Aubert, P. Pale, A. Tkatchenko, J.-P. Djukic, and V. Mamane, Chem. Eur. J. **30**, e202302933 (2023)

Molecules in Environments: Toward Systematic Quantum Embedding of Electrons and Drude Oscillators
M. Ditte, M. Barborini, and A. Tkatchenko, Phys. Rev. Lett. **131**, 228001 (2023)

Fractional charge by fixed-node diffusion Monte Carlo simulation
M. Ditte and M. Dubeck, Phys. Rev. Lett. **123**, 156402 (2019)

Toward Accurate Hydrogen Bonds by Scalable Quantum Monte Carlo
M. Dubecký, P. Jurečka, L. Mitas, M. Ditte, and R. Fanta, J. Chem. Theory Comput. **15**, 3552 (2019)

SELECTED CONFERENCES

17th International Congress of Quantum Chemistry (ICQC2023) *Jun.-Jul. 2023*

Psi-k Conference 2022 *Aug. 2022*

Recent developments in quantum Monte Carlo (CECAM) *Oct. 2021*

Non-Covalent Interactions in Large Molecules and Extended Materials (CECAM) *Aug.-Sep. 2021*

APS March Meeting 2021 *Mar. 2021*

SELECTED TRAINING

TREX e-School on Quantum Monte Carlo with TurboRVB *Jul. 2021*

ULHPC School 2020 *Dec. 2020*

Quantum Monte Carlo and the CASINO program X, Vallico Sotto *Jul. 2016*

AWARDS AND HONORS

Diploma of Excellence, 2019

LANGUAGES

English	C1
Slovak	native

TECHNICAL SKILLS

Programming Languages	C++, Fortran, Python, Bash script
Numerical Mathematics	Mathematica, Matlab
Quantum Chemistry Codes	QMCPack, QWalk, QMeCha, GAMESS, Gaussian, Psi4, PySCF, Orca, FHI-aims, Quantum Espresso