MSCA PF 2026 HOSTING OFFER

Name of the host institution	*Budapest University of Technology and Economics*
Faculty	*Faculty of Chemical Technology and Biotechnology*
Name of the supervisor	*Péter Nagy*
Organisational Unit / Research Group	*ERC Molecular Quantum Simulation Research Group*
Research Team	*Team members: PI, 4 postdoc, 3 PhD, 3 undergraduate: http://www.fkt.bme.hu/~theoreticalchem/index.php/group* *Expertise: development of quantum chemistry models and programs with universally trusted predictive power and their acceleration to routinely affordable simulation times. Modeling and understanding of complicated molecular interactions and reactions that are not accessible accurately without our models, including drug-protein, supramolecules, molecular crystals, and reactivity across homogeneous, surface and enzyme catalysis.*
Project experiences (EU / international)	*European Research Council (ERC) project 2023 aCCuracy:* *Turning gold standard quantum chemistry into a routine simulation tool: predictive properties for large molecular systems* *MSCA PF project 2025 DNACopyComp:* *Development of a predictive quantum simulation protocol for understanding DNA polymerase function and toxic inhibition* *MSCA cofund project 2025:* *Development of a broadly predictive quantum model applicable to practical transition-metal catalysis: understanding CO2 reduction* *MSCA cofund project 2026:* *Harnessing gold-standard predictive power for solid-state batteries: Optimization of the conductivity and polymerization catalysts for polymer electrolytes*
Research Interests	*Predictive modeling and atomistic understanding of challenging covalent- and non-covalent interactions in large molecules using our models, where modern workhorse computational methods (such as DFT) have well-known difficulties:* *1) complicated interactions between large molecules governing, e.g., supramolecular and catalyst-substrate interactions. E.g., protein-drug interactions and molecular crsytals.* *2) the mechanism of environment-friendly and selective organo-, and earth-abundant transition-metal catalytic reactions. E.g., CO_2, H_2O, and N_2 activation.* *3) surface and enzyme catalysis in proper solvent, crystal, and*

	protein environment. E.g., computational mechanistic study of phosphate reactions relevant to cancer formation or human DNA and viral RNA polymerization and related drug design. *Development of quantum chemistry models and programs:* *4) improving the accuracy and speed of our methods via better approximations (via, e.g., higher-order perturbative estimates, explicit electron correlation, improved long-range interactions, etc.) and a massively parallel code* *5) development and practical implementation of similarly efficient DFT and local CCSD(T) level observables, such as thermodynamic, structural, spectroscopic, and dynamic molecular properties* *6) Further development and application of our multilevel or embedding methods using gold standard accuracy for the chemically active region combined with cost-efficient models (MP2, DFT, ML, MM) to take into account biochemical, crystal, and solvent environment effects.* *7) Blending wavefunction and DFT methods to extend and improve our double-hybrid and wavefunction-in-DFT embedding approaches* *8) Extensions of these efficient and accurate DFT, PT, and CC methods to open-shell and multireference systems.* *Detailed project description:* *www.fkt.bme.hu/~theoreticalchem/index.php/open-positions*
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