Theoretical Chemistry Group - TCG

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At TCG we develop theoretical models and computational simulations of molecular properties and reactivity. We address a wide range of physical chemistry topics, from magnetic and optical spectroscopies to the design of functional molecular structures using molecular dynamics, quantum-statistical and stochastic thermodynamics methods. We investigate also novel approaches, like machine learning techniques and quantum technologies, for theoretical and computational chemistry. Current research subjects are:

- coarse-grained description of biomolecules and supramolecular systems
- deterministic and stochastic kinetics in chemical reaction networks
- computer-guided rational design of bio inspired molecules and catalysts for applications to health and sustainability
- design of quantum nanodevices for molecular logic
- models of quantum dynamics and spectroscopic response

1. Strategies to simulate dephasing-assisted quantum transport on digital quantum computers. New Journal of Physics 2022, 24, 023039.
2. Effect of methylmercury binding on the peroxide reduction potential of cysteine and selenocysteine. Inorg. Chem. 2021, 60, 4646-4656.
3. Stochastic modelling of C-13 NMR spin relaxation experiments in oligosaccharides. Molecules 2021, 26, 2418
4. Sensitivity analysis of the reaction occurrence and recurrence times in steady-state biochemical networks. Math. Biosci. 2021, 333, 108518
5. Parameter free evaluation of SN2 reaction rates for halide substitution in halometane. Phys. Chem. Chem. Phys. 2022, 24, 7474.