Theoretical Chemistry

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The Theoretical Chemistry group is active in several areas of theoretical and computational chemistry, including the interpretation of magnetic and optical spectroscopies, the modeling and *in silico* investigation of materials and functional molecular structures, molecular dynamics of macromolecules, microfluidics, quantum-statistical and stochastic thermodynamics. Current subjects of investigation are:

- coarse-grained description of biomolecules and supramolecular aggregates;
- multiscale methods for the self-assembly of large molecular systems;
- design of quantum nanodevices for molecular logic and sensing;
- dynamics and statistics of open quantum systems;
- dimensional reduction of complex chemical reaction networks;
- rational design of semi-natural enzymes, bio inspired drugs and catalysts.

- *Integrated computational approach to the Electron Paramagnetic Resonance characterization of rigid 310-helical peptides with TOAC nitroxide spin labels,* J. Phys. Chem. B*,* **2017***,* 121, 4379-4387.
- *The quantum molecular trajectory and its statistical properties*, J. Phys. Chem. A*,* **2017***,* 121, 5352-5360.
- *Addition-elimination or nucleophilic substitution? Understanding the energy profiles for the reaction of chalcogenolates with dichalcogenides,* J. Chem. Theory Comput.*,* **2016***,* 12, 2752-2761.
- *A low-computational-cost strategy to localize points in the slow manifold proximity for isothermal chemical kinetics*, Int. J. Chem. Kinet.*,* **2017***,* 49, 477-493.
- *A probabilistic finite state logic machine realized experimentally on a single dopant atom,* Nano Letters*,* **2017***,* 17, 1846-1852.