Research outputs:

**Excited-state solvation structure of transition metal complexes from molecular dynamics simulations and assessment of partial atomic charge methods**
Research output: Research - peer-review › Journal article – Annual report year: 2019

**Theoretical Evidence of Solvent-Mediated Excited-State Dynamics in a Functionalized Iron Sensitizer**
Research output: Research - peer-review › Journal article – Annual report year: 2019

**Anisotropy enhanced X-ray scattering from solvated transition metal complexes**
Research output: Research - peer-review › Journal article – Annual report year: 2018

**Photoinduced Molecular Dynamics in Solution: Multiscale Modelling and the Link to Ultrafast Experiments**
Research output: Research › Ph.D. thesis – Annual report year: 2018

**Solution Structure and Ultrafast Vibrational Relaxation of the PtPOP Complex Revealed by ΔSCF-QM/MM Direct Dynamics Simulations**
Research output: Research - peer-review › Journal article – Annual report year: 2018

**Mechanism and Thermochemistry of Coal Char Oxidation and Desorption of Surface Oxides**
Research output: Research - peer-review › Journal article – Annual report year: 2017

**Grid-Based Projector Augmented Wave (GPAW) Implementation of Quantum Mechanics/Molecular Mechanics (QM/MM) Electrostatic Embedding and Application to a Solvated Diplatinum Complex**
Research output: Research - peer-review › Journal article – Annual report year: 2017

Projects:

**Light-induced electronic and structural dynamics**
Project: PhD