Research outputs:

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

**Dissociation, absorption and ionization of some important sulfur oxoanions (S\(_2\)O\(_n\)\(^{2-}\) n = 2, 3, 4, 6, 7 and 8)**
Research output: Research - peer-review › Journal article – Annual report year: 2015

**Prediction of acidity constants of some important selenium oxoacids in aqueous solution by computational techniques**
Research output: Research - peer-review › Journal article – Annual report year: 2014

**Acidity constants of some sulfur oxoacids in aqueous solution using CCSD and MP2 methods**
Research output: Research - peer-review › Journal article – Annual report year: 2013

**Theoretical studies on the tautomerism of tetrazole selenone**
Research output: Research - peer-review › Journal article – Annual report year: 2013

**Theoretical study on the mechanism and kinetics of acetaldehyde and hydroperoxyl radical: An important atmospheric reaction**
Research output: Research - peer-review › Journal article – Annual report year: 2013

**Theoretical study on the structures, stabilities and electronic properties of S\(_2\)O\(_5\)\(^{2-}\) isomers in the gas and solution phases**
Research output: Research - peer-review › Journal article – Annual report year: 2013

Projects:

**Atomistic Mechanisms of Functional Molecules**
Project: PhD