Report: Automatic Exploration of Excited-State Reactive Events

Subject: Short Term Scientific Mission
Applicant: Patrick Zobel, University of Vienna Reference: COST Action CM1405
Host Institution: Group of Prof. Emilio Martínez Núñez, University of Santiago
Period: 05/09/2016 to 30/09/2016
Reference code: COST-STSM-ECOST-STSM-CM1405-050916-079928

Dear Sir or Madam,

here I report the tasks that I have accomplished during my STSM in the group of Prof. Emilio Martínez Núñez at the University of Santiago. The main goal of the STSM was to extend the existing transition state search using chemical dynamics simulations (TSSCDS) code of Prof. Martínez, which was developed to be used for the electronic ground state, to be used for excited states, too, and to apply the extended TSSCDS in the investigation of the excited-state reactions of nitrobenzene (NB). TSSCDS first calculates transition states (TS) and minimum-energy paths (MEP) at a low level of theory (LL), e.g., using classical molecular mechanics, and then refines the results at a higher level of theory (HL), e.g., using density functional theory (DFT). Before the STSM, already LL test calculations were conducted–in this case at the configuration interaction singles (CIS) level of theory –to identify TSs and MEPs of NB. As the first STSM task, it was planned to interface the TSSCDS code to run with the quantum chemistry program TERACHEM. To locate transition states, TERACHEM is only able to use the nudged-elastic band (NEB) method, which does not start at the TS but rather connects two energetic minima by a MEP thus trying to find the TS. Test calculations attempting to find TSs at HL (time-dependent DFT) using the NEB method starting from structures close to the TSs found at LL, however, proved to be quite inefficient. Therefore, it was decided instead to interface TSSCDS to the TURBOMOLE program package. This task was succesfully completed and a working version of TSSCDS/TURBOMOLE exists at the cluster at the Institute of Theoretical Chemistry in Vienna. This version was then used to start the study of the excited-state reactions of NB for the remainder of the STSM. Thus, TSSCDS calculations for the first excited singlet state (S_1) of NB were run and promising results were achieved, e.g., location of more the 50 TS in the S_1 of NB. The future work now includes the application of TSSCDS to other excited states of NB. Additionally, to obtain a more complete picture of the possible reaction channels, TSSCDS calculations will also be run for the ground state of NB. For consistency, this should be done at the same level of theory as for the excited state which requires further small modifications of the TSSCDS/TURBOMOLE interface.

Yours sincerely,

Patrick Zobel (Vienna, October-24, 2016)

Confirmation of the host of the successful execution of the STSM

I confirm that Patrick Zobel from University of Vienna worked at the University of Santiago from 05/09/2016 to 30/09/2016. The visit has been successful and the results obtained are described above.

Prof. Emilio Martínez Núñez (Santiago, October-24, 2016)