List of completed scientific and professional international visits

2013 – 2016 Independent researcher & Postdoctoral researcher & Software developer,
University of Jena, Germany & TURBOMOLE GmbH, Germany.
(3 years and 2 months)

As independent researcher awarded DFG grant No. 269386423 on development of tool for global structure optimization of clusters in confined spaces (10.1021/acs.jpcc.6b09423). As postdoctoral researcher implementing analytical gradients for new periodic density functional theory module RIPER in TURBOMOLE program. As a software developer development of a low-memory density fitting approximation in quantum chemical calculations (10.1002/jcc.23961) and Hybrid MPI+OpenMP parallelization of the Fortran legacy code in the proprietary TURBOMOLE quantum chemistry package.

07/2011 **Visiting researcher,** *University of Pittsburgh, USA (with Prof. K. D. Jordan)* (2 weeks)

Within the Czech American cooperation project (Amvis - CONTACT, ME10032) dealing with a accurate description of gas adsorption in nanoporous materials.

04/2011 **Visiting researcher,** *University of Edinburgh, UK (with Prof. T. Düren)* (1 week)

Within MACADEMIA Project (FP7-NMP-2008-LARGE-2 project No. 228862). Development of the ab initio-based representation of potential energy surface for accurate description of adsorption using grand canonical Monte Carlo simulation. The visit was part of collaboration on a joined topic which resulted in a joint publication (10.1021/jp2090878).

07-09/2008 **Research student,** *Humboldt University, Berlin, Germany (with Prof. J. Sauer)* (3 months)

Gained expertise in hybrid quantum-mechanics/molecular-mechanics simulations.