

JAN CHALABALA

chalabaj@vscht.cz

RESEARCH INTEREST

I focus on quantum chemistry and molecular dynamics simulations of radiation processes in hydrogen bonded systems with relevance to astrochemistry.

EDUCATION

International Max Planck Research School, Dresden (joint Ph.D.) 2015-now
University of Chemistry and Technology, Prague

Ph.D. Physical chemistry

Dissertation: X-ray photodynamics: molecular simulation of radiation processes

University of Chemistry and Technology, Prague 2010-2015

M.Sc. Molecular analytical and physical chemistry (*summa cum laude*)

Thesis: Intermolecular interactions of aromatic compounds in excited and ionized states

B.Sc. Environmental Chemistry and Toxicology (*summa cum laude*)

Thesis: Influence of bicarbonate ion on carbon steel corrosion

WORK EXPERIENCE

University of Chemistry and Technology, Prague 09/2015-now
assistant at Department of physical chemistry

Institute of Chemical Process Fundamentals of the ASCR 04/2014
short-term internship
processing gas chromatography spectra

Department of Petroleum Technology, UCT Prague 06 - 08/2012
short-term internship
developing procedure for image analysis of particles in oil sediments

Arkon flow systems s.r.o., Brno 06 - 09/2009
constructing electromagnetic flow meters for foreign customers
final testing and calibrating devices before delivery

CERTIFICATES AND COURSES

Astrochemistry: from space to Earth summer school 2016
University of Grenoble, Grenoble

ATHENS programme

Climate change and ethics, University of Technology, Delft 2015

Safety Engineering, Katholieke Universiteit, Leuven 2014

Nanotechnologies, Ecole Nationale Supérieure de Techniques Avancées, Paris 2013

Arctic technology field course 2013

Technical University of Denmark, Greenland

Installation and measurement of micro-hydro power plant in arctic conditions

Introduction to solid state chemistry course 2013

Massachusetts Institute of Technology, Cambridge

Astronomy 2013-2014

Prague planetarium and Stefanik Observatory, Prague

Two-years seminar with sky observations

ADDITIONAL SKILLS

Computer: MS Office, Linux (user), HTML/CSS/, Bash/Fortran/Python (basics), GitHub(user)

Specialized: Quantum chemistry packages (Gaussian, MOLPRO, Q-CHEM, OCTOPUS),
Mathematica (basics),

Language: English (B2+)

Driving license class B

LIST OF PUBLICATIONS

Papers

- Chalabala, J.; Slavíček, P.: Nonadiabatic dynamics of floppy hydrogen bonded complexes: the case of the ionized ammonia dimer, *Phys. Chem. Chem. Phys.*, 2016, **18**, 20422-20432

Posters

- Chalabala, J.; Slavíček, P.: Structure and Dynamics of Ionized Ammonia Dimer. 51st Symposium on Theoretical Chemistry, Potsdam, 2015
- Chalabala, J.; Slavíček, P.: Radiation Chemistry of Water Dimer with Real-Time TDDFT, 17th European Seminar on Computational Methods in quantum Chemistry, Shropire, 2017.

Given talk

- Chalabala J., Macak J.: *Influence of bicarbonate ions on carbon steel corrosion*.
Conference collection „Chemie energetických okruhu 9“, p40, Prague, 2012

RECEIVED GRANTS & AWARDS

Wiley outstanding poster award 2017

17th European Seminar on Computational Methods in quantum Chemistry, Shropire

Postgraduate university research grant 2016, 2017

University of Chemistry and Technology, Prague

Development of a code for wavefunction based Ehrenfest molecular dynamics