Research Associate in Computational Chemistry

Holds the position from 12.11.2013

Dr. Paweł Rejmak

FIELD OF EXPERTISE
Simulations of molecules and solids by means of density functional theory and molecular mechanics.

EDUCATION

- Msc: in Quantum Chemistry (with honors), Dept. of Chemistry, Maria Curie-Sklodowska University, Lublin, Poland, 2003.
- PhD in Quantum Chemistry (with honors), Institute of Catalysis and Surface Chemistry PAS, Krakow, Poland, 2008.

EXPERIENCE

- 2009–2010 Assistant in Institute of Catalysis and Surface Chemistry PAS.
- 2010–2013 Post-Doctoral Researcher, Donostia International Physics Center, Donostia-San Sebastian, Spain.

Dr. Paweł Rejmak is currently a researcher in the Institute of Physics PAS. He is experienced in the applications of various computational chemistry methods for simulation of applied materials, such as zeolite based catalysts and cements, usually in close collaboration with experiments.
Within EAgLE project of Dr. Rejmak focus on modeling and computational characterization of a new metalorganic compounds for biological and medical applications. The theoretical data about structural, electronic and spectroscopic properties of these compounds should give complement data achieved from experiments performed in the group of X-ray Spectroscopy and Microanalysis.

Selected publications

1. A. Cuesta, A. G. de la Torre, E. R. Losilla, V. K. Peterson, **P. Rejmak**, A. Ayuela, C. Frontera, M. A. Aranda "Structure, Atomistic Simulations, and Phase Transition of Stoichiometric Yeelimite", *Chem. Mater. 25* (2013*)* 1680.
2. **P. Rejmak**, J. S. Dolado, M. S. Stott, A. Ayuela, "29Si Chemical Shift Anisotropies in Hydrated Calcium Silicates: A Computational Study", *J. Phys. Chem. C*, *117* (2013) 8374.
3. **P. Rejmak**, J. S. Dolado, M. S. Stott, A. Ayuela, "29Si NMR in Cement: A Theoretical Study on Calcium Silicate Hydrates", *J. Phys. Chem. C*, *116* (2012) 9755.
4. **P. Rejmak**, M. Mitoraj, E. Broclawik, „ Electronic View on Ethene Adsorption in Cu(I) Exchanged Zeolites", *Phys. Chem. Chem. Phys.*, 12 (2010) 2321.
5. **P. Rejmak**, E. Broclawik, M. Radon, K. Góra-Marek, J. Datka, „Nitrogen Monoxide Interaction with Cu(I) Sites in X and Y Zeolites: Quantum Chemical Calculations and IR Studies", *J. Phys. Chem.C*, 112 (2008) 17998
6. **P. Rejmak**, M. Sierka, J. Sauer, „Theoretical Studies of Cu(I) Sites in Fauajsite and Their Interaction with Carbon Monoxide", *Phys. Chem. Chem. Phys.*,9 (2007) 5446.