NANOSCIENCE AND NANOTECHNOLOGY PROGRAM

Andreas Köster, Dr. habil.

Research Interests

- Ab-Initio Electronic Structure Methods
- Density Functional Theory
- Quantum Chemical Program Development (deMon2k)
- Molecular Property Calculations
- Born-Oppenheimer Molecular Dynamics
- Cluster Science & Nanoscience
- Transition Metal Chemistry

Dr. Köster is Professor in the Department of Chemistry at Cinvestav. In 1992 he earned his PhD from the Leibniz Universität Hannover in Chemistry under the supervision of Prof. Dr. Jug. After a post-doctoral stay (1993-1994) with Prof. Dr. Salahub at the Université de Montréal he started his habilitation in Theoretical Chemistry in 1995. It was awarded to him in 1998 by obtaining the venia legendi (permission to read, i.e. to lecture) for Theoretical Chemistry. Between 1998 and 1999 he was hired as Priv.-Doz. at the Leibniz Universität Hannover. At the end of 1999 he followed a call from Cinvestav where he took the position of Investigador Titular in the Department of Chemistry. Since 2012 he also is member of the institutional PhD program in Nanoscience and Nanotechology.
Dr. Köster has authored or co-authored more than 100 peer reviewed research publications that received over 3000 citations. He also contributed to more than 10 book chapters and has delivered around 100 invited talks at international conferences. He is principal author of the density functional theory program deMon2k which is distributed to around 400 research groups all over the world. His research interest is in the development and application of first-principle electronic structure method to complex molecular systems.

Selected Honours and Awards

- SNI III since 2010

Research Project: QM/MM Study of the Melting of Lipid Bilayers

The melting of lipid bilayer structures is of fundamental importance for the functioning of cell membranes. It has also large applications in pharmaceutical chemistry. The here proposed research aims to gain insight into this melting process by a multiscale approach that combines first-principle quantum mechanical (QM) and molecular mechanics (MM) methodologies. To this end we plan QM/MM calculations with the program deMon2k [1] on lipid bilayer model systems employing a combination of Born-Oppenheimer [2] and classical molecular dynamics simulations [3]. The proposed research work consists of development and application tasks including the construction of an appropriate atomistic model for lipid bilayers. The successful applicant should have a master degree in Chemistry, Physics or a related area. Scientific programming experience is advantageous but not a must.

[1] See www.deMon-software.com
[2] J.M. Vásquez-Pérez et al., *J. Phys. Chem. Lett.* **6**, 4646 (2015)
[3] D.R. Salahub et al. *Molecules*, **20**, 4780 (2015)