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 120 peer reviewed research publications that received around 4000 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 COVID-19 Proteases

Attractive drug targets against coronaviruses are their main proteases (M^{PRO} also called $3CL^{PRO}$) due to their critical role in processing polyproteins that are translated from the viral RNA. The M^{PRO} is involved in at least 11 cleavages and prune to mutations. Inhibiting this enzyme will block viral replication. Since no human proteases with similar cleavage specificity are known, inhibitors are unlikely to be toxic to humans. Therefore, the molecular and electronic structures of these proteases are of great importance for the rational design of new antiviral drugs against COVID-19.
The here proposed research aims to gain insight into the inhibition of COVID-19 M^{PRO}s by a multiscale approach that combines first-principle quantum mechanical (QM) and molecular mechanics (MM) methodologies. To this end, we plan QM/MM calculations [1,2] with the program deMon2k [3] on COVID-19 M^{PRO}s and corresponding inhibitors. The proposed research work consists of development and application tasks including the construction of an appropriate atomistic model for COVID-19 M^{PRO}s. 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] D.R. Salahub et al. *Molecules*, **20**, 4780 (2015)
[2] A. de la Lande et al. *Molecules*, **24**, 1653 (2019)
[3] See www.deMon-software.com