Post-doc position: Ab initio free energy calculations for molecule – surface interactions with chemical accuracy

available immediately and limited to 11/2020 (project end).

To achieve chemical accuracy for molecule – surface interactions (Piccini et al., Angew Chem Int Ed 54, *2016*, 5235; Piccini et al. J Phys Chem C 119, *2015*, 6128) a method has been developed to calculate vibrational partition functions using anharmonic vibrational energies. The latter are obtained by solving 3N one-dimensional vibrational problems (see: Piccini & Sauer, J Chem Theory Comput, 10, *2014*, 2479). The post-doc is expected to further develop the methodology into robust protocols, for example by identifying
(i) subspaces of normal modes for which anharmonicities can be obtained by simple scaling
(ii) subspaces that correspond to rigid body motions relative to the surfaces
(iii) modes that involve internal rotations.

The task involves programming, testing and challenging applications as well as comparison with free energy simulations by Monte Carlo methods and Molecular Dynamics. Candidates are expected to have a PhD in Theoretical Chemistry/Physics, programming skills and profound knowledge of quantum chemical methodology in particular for nuclear motions in anharmonic potentials.

Applications by email (js@chemie.hu-berlin.de) to

Professor Joachim Sauer, Institut für Chemie, Humboldt-Universität zu Berlin
(www.chemie.hu-berlin.de/de/forschung/quantenchemie)