Grand-Canonical-like adaptive resolution model for molecules with electrons

Requested start date

1.7.2023

Type of proposal

Initial proposal

Whitelist

DFG project (Project Number 439321740, start in 2020 - proposal was put to a pause in 2022, therefore it has been extended till 2024)

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DFG classification (RB-Nr.)

327-01 Theoretical Chemistry: Electron Structure, Dynamics, Simulation

Short abstract

The goal of this project is to simulate the quantum/classical (QM/MM) large-scale molecular systems, in which molecules can switch from a quantum region to a classically treated environment, depending on their position in the simulation space. The idea is based on the Grand Canonical description of a quantum region embedded in a classical reservoir of molecules. Electronic properties of the quantum region are calculated at constant electronic chemical potential equal to that of the corresponding large reference system reference treated at full quantum level. In addition, the Grand Canonical Adaptive Resolution Scheme (AdResS) is used for the treatment of the classical environment, and the exchange of molecules between the QM and MM parts occurs at the chemical potential of the macroscopic thermodynamic conditions. Finally, the method is applied to an important problem in physical chemistry: the calculation of the adsorption energy of phenylalanine (in aqueous solution) on a metallic Pt(111) surface.