Combined ab initio/semi-empirical Screening Protocol for Properties of Self-Assembled Monolayers

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Organic electronic devices recently found their way into the first consumer products such as mobile phone displays. These devices take advantage of the unique properties of organic materials such as transparency, flexibility, and simple and low-cost processability. However, they always need to be incorporated into conventional inorganic electronic frameworks. This very often leads to a lower device performance and limit the choice of materials.

Self-assembled monolayers (SAMs) are a means to improve the organic-inorganic junction: dipolar organic molecules form an interlayer between the inorganic electrode and the organic semiconductor, tune the effective work function of the electrodes and adjust the metal's Fermi energy to the conduction bands of the organic semiconductor.

For a well-directed synthesis of SAMs, computational screening methods are necessary in order to search for organic molecules with given properties. The prediction of SAM-properties is possible with reasonable accuracy using plane-wave density functional theory calculations. However, the costs of these methods are too high to allow systematic in silico searches for new materials.

Here, we present a combined *ab initio*/semi-empirical protocol for predicting properties of SAMs. Taking advantage of restricted semi-empirical geometry optimizations reduces the total computation time for work-functions by more than one order of magnitude. In all cases periodic boundary conditions are taken into account.

The protocol was successfully applied to more than 15 functionalized thiols on gold and silver surfaces. Finally the robustness of the methodology was evaluated comparing the calculated work functions with experimental data.