Benchmark Database of Transition Metal Surface and Adsorption Energies from Many-Body Perturbation Theory - DTU Orbit (19/11/2018)

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We present an extensive set of surface and chemisorption energies calculated using state of the art many body perturbation theory. In the first part of the paper we consider 10 surface reactions in the low coverage regime where experimental data is available. Here the random phase approximation (RPA) is found to yield high accuracy for both adsorption and surface energies. In contrast, all the considered density functionals fail to describe both quantities accurately. This establishes the RPA as a universally accurate method for surface science. In the second part, we use the RPA to construct a database of 200 high quality adsorption energies for reactions involving OH, CH, NO, CO, N-2, N, O, and H over a wide range of 3d, 4d, and 5d transition metals. Due to the significant computational demand, these results are obtained in the high coverage regime where adsorbate adsorbate interactions can be significant. RPA is compared to the more advanced renormalized adiabatic LDA (rALDA) method for a subset of the reactions, and they are found to describe the adsorbate-metal bond as well as adsorbate-adsorbate interactions similarly. The RPA results are compared to a range of standard density functional theory methods typically employed for surface reactions representing the various rungs on Jacob’s ladder. The deviations are found to be highly functional, surface, and reaction dependent. Our work establishes the RPA and rALDA methods as universally accurate full ab initio methods for surface science where accurate experimental data is scarce. The database is freely available via the Computational Materials Repository (CMR).

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