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"QM/Me" - a novel embedding approach for adsorbate dynamics on metal surfaces JÖRG MEYER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, KARSTEN REUTER, TU Muenchen — The dissociative adsorption of oxygen molecules on metal surfaces is a commonly known, highly exothermic reaction and in its slow or fast form of great importance for corrosion or oxidation catalysis, respectively. However, knowledge about atomistic details of the heat dissipation, a central conceptual concern, is very limited at best. Even on the level of Born-Oppenheimer potential energy surfaces, accurate dynamical *ab-initio* descriptions of such reactions are quite challenging from a computational point of view: Modeling the excitations of substrate phonons within periodic boundary conditions requires huge supercells, whereas traditional "QM/MM" embedding schemes would need unfeasibly large metal clusters. In the novel "QM/Me" approach presented here, the adsorbate- interaction is obtained from periodic first-principles calculations in convenient supercells and combined with the description of a 'bath-like' substrate based on classical potentials, which are parametrized to seamlessly fit the first-principles data. We apply our approach to the dissociative adsorption of O_2 and H_2 on Pd(100) using density-functional theory and a modified embedded atom potential. In both cases, a dominant fraction of the released chemisorption energy is dissipated into the bulk already on a femtosecond time scale. Implications for the adsorbate dynamics will be discussed.

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