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Surface chemistry in a full-potential QM/MM approach: making hybrids affordable DANIEL BERGER, Technical University Munich, VOLKER BLUM, Fritz-Haber-Institut der MPG, Berlin, KARSTEN REUTER, Technical University Munich — Nanostructured oxide surfaces are promising candidates for a wide range of energy and catalysis applications. When addressing corresponding functionalities through quantitative first-principles calculations, exploitation of the localized character of the chemical processes yields numerically most efficient approaches. To this end we augment the FHI-aims[1] package with a QM/MM[2] functionality, in which the nanostructure and immediate oxide surrounding is described quantum mechanically, the long-range electrostatic interactions with the support are accounted for through a polarizable monopole field, and a shell of norm-conserving pseudopotentials correctly connects the two regions. We illustrate the accuracy and efficiency of the implementation with examples from the photo-catalytic water splitting context and specifically discuss the use of charged system states to address charge transfer processes.

[1]V. Blum *et al.*, Comput. Phys. Commun., **180**, 2175-2196 (2009)
[2]N. Bernstein *et al.*, Rep. Prog. Phys., **72**, 026501 (2009)

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