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A quantum chemistry roadmap towards highly accurate adsorption energies at ionic surfaces BO LI, Fritz-Haber-Institut der Max-Planck-Gesellschaft, ANGELOS MICHAELIDES, London Centre for Nanotechnology, University College London and Fritz-Haber-Institut der Max-Planck-Gesellschaft, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft — A roadmap is established to compute adsorption energies of molecules at ionic surfaces with an accuracy approaching chemical accuracy (a precision of 1 kcal/mol or ∼43 meV). The approach relies on established quantum chemistry methodologies and involves a separation of the total adsorption energy into contributions from Hartree-Fock and electron correlation, the use of embedded cluster models of the substrate, and extrapolations to the complete basis set limit. Application of the procedure to the example of water on salt, with electron correlation treated at the CCSD(T) level, yields an adsorption energy for a water monomer on NaCl(001) of 480 ± 20 meV.

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