Embedded cluster calculations on adsorption at oxide surfaces

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In the field of heterogeneous catalysis the great majority of quantum chemical calculations are nowadays DFT (density functional theory) slab calculations using periodic boundary conditions and plain wave basis sets.

For local processes such as adsorption, the embedded cluster approach (Fig. 1) is an alternative approach allowing for the usage of higher level quantum chemical methods [DFT with hybrid functionals, MP2 perturbation theory, and coupled cluster singles and doubles with perturbative triples (CCSD(T))] to benchmark the accuracy of the plane wave calculations.

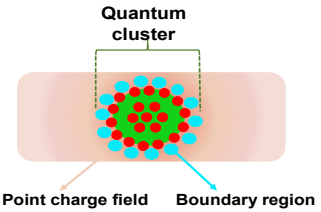

Figure 1: Embedded cluster approach

For the example**s** of CO adsorbed on alumina **(α-Al_2O_3)** and ceria **(CeO_2)**, we compare the adsorption energy and stretching vibrational frequency of CO obtained by different computational methods and by experiment. We discuss the accuracy of the different approaches and their applicability for different experimental conditions.