Czech Chemical Society Lecture

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Towards reliable calcula ions of binding energies of molecular solids

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Binding energies of molecular clusters and solids are one of their important properties. There is thus a range of theoretical methods that can be used to calculate the binding energy and that differ in their accuracy and computational cost. I will discuss some of the methods and show their applications to determining stability of experimentally observed structures. Primarily I will present results for the random phase approximation which is a method that, in terms of accuracy and computational demands, sits between reference quality coupled clusters methods and widely used density functional theory approaches. I will focus on how we can understand in detail the results that the various methods give for binding energies using methane clathrate and crystals of small molecules. Finally, I will discuss results obtained using even simpler classical force fields for systems involving water and graphene in collaboration with experimentalists.