Recent progress in applying periodic coupled cluster theory to solids and surfaces

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This presentation will review recent progress in applying periodic coupled cluster theory to *ab initio* studies of solids and surfaces. We will discuss techniques that reduce the computational cost by accelerating the convergence of calculated properties towards the complete basis set as well as the thermodynamic limit using a plane wave basis [1-3]. We will present a diagrammatic decomposition of the coupled cluster correlation energy that makes it possible to correct for the basis set incompleteness error in a computationally efficient manner [1]. These developments have enabled an increasing number of *ab initio* studies and allowed for assessing the accuracy of coupled cluster theories by comparing to experimental findings as well as quantum Monte Carlo results. The presented applications will include phase transitions of solids [4] and molecular adsorption energies [5-7].

References

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