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Towards efficient coupled-cluster theories for periodic systems

THEODOROS TSATSOULIS, FELIX HUMMEL, ANDREAS GRUENEIS, Max Planck Institute for Solid State Research — Over the last few years, quantum-chemical correlation methods have been increasingly often applied on extended systems. In this work we consider an ab-initio description of the true many-body wave function. We explore canonical coupled-cluster theory within the projector-augmented-wave method in a plane-wave basis. A combination of Gaussian basis-functions with plane-waves, as well as a low-rank factorization of the Coulomb integrals results in an effective quantum-chemical scheme for extended systems. We demonstrate the capabilities of the methods by studying molecular interactions with periodic surfaces.

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