Ground-state properties of metals from coupled-cluster theory

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Coupled-cluster theory is known to provide "chemical accuracy" in molecules and has more recently been applied to insulating solids. However, the application of coupled-cluster theory to atomistic metals is relatively unexplored. Using optimized basis sets, we evaluated the lattice constant, bulk modulus, and cohesive energy of aluminium and lithium with coupled-cluster theory with single and double excitations (CCSD). We observe reasonable accuracy that is competitive with that from common density functionals. We considered two strategies beyond CCSD, which were found to improve the accuracy: adding coarse grained perturbative triples contributions and scaling the valence CCSD correlation energy using its error in the uniform electron gas, a model metallic system.

See VAN, H.-Z. Ye, T. C. Berkelbach, arXiv:2204.01563.