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The role of vdW interactions for the cohesive properties of the coinage metals LORENZ ROMANER, Chair of Atomistic Modelling and Design of Materials, University of Leoben, A-8700 Leoben, Austria., MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, 14195 Berlin, Germany, CLAUDIA AMBROSCH-DRAXL, Chair of Atomistic Modelling and Design of Materials, University of Leoben, A-8700 Leoben, Austria. — Density-functional theory has been successfully applied over many years to calculate binding energies and bond lengths for a wide range of systems. More recently, it has been extended to include long-range correlation interactions and hence could be used for purely van der Waals (vdW) bound systems such as noble gas solids or organic crystals. On the other hand, early calculations for noble metals have revealed a vdW contribution to the cohesive energy [Rehr, Zaremba, Kohn, PRB 12, 2062 (1975)]. We investigate this issue by employing the vdW-DF approach [Dion et al., PRL 92, 296401 (2004)], where the exchange interactions are treated within revPBE, and the non-local correlations are based on an approximation to the adiabatic connection formula. We find that the latter give a substantial contribution to the cohesive energies but, overall, vdW-DF underestimates their magnitude while overestimating the lattice parameters. We attribute this shortcoming to the local part of the correlation energy.

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