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Extended disperson-corrected atom-centered potential (DCACP) approach for treating long-range dispersion interactions in clusters and solids[1] KENNETH JORDAN, OZAN KARALTI, WISSAM AL-SAIDI, University of Pittsburgh — The DCACP method of Rothlisberger and co-workers[1] is one of several strategies for correcting density functional theory for dispersion interactions. The DCACP approach, which involves the use of additional terms in standard pseudopotentials, has proven very successful near the potential energy minima of molecular dimers but gives an interaction energy that falls off much too rapidly as the separation between the monomers is increased. In our work, we extend the DCACP approach for H, C, N, and O to include two angular momenta channels in the pseudopotentials rather than one in the original DCACP method (an idea originally explored by Rothlisberger for $(H_2)_2$).[2] We show that this approach, which we designate as DCACP2, significantly improves the description of long-range dispersion interactions. [1] O. A. von Lilienfeld, I. Tavernelli, U. Rothlisberger, and D. Sebastiani, Phys. Rev. Lett., 93, 153004. (2004). [2] I. Tavernelli, I.-C. Lin, and U. Rothlisberger, Phys. Rev. B, 79, 045106, (2009).

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