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Hybrid functional pseudopotentials JING YANG, LIANG Z. TAN, ANDREW M. RAPPE, Univ of Pennsylvania, THE MAKINENI THEORETICAL LABORATORIES TEAM — The consistency of exchange-correlation functionals used in pseudopotential construction and the actual density functional theory calculation can affect the accuracy of geometric parameters and band gaps of chemical species. However, routine hybrid functional calculations at present use GGA pseudopotentials instead of pseudopotentials constructed from hybrid functional all-electron calculations, because of the lack of a publicly available hybrid functional pseudopotential generator. The mismatch of exchange-correlation functionals between pseudopotential and DFT calculations could lead to systematic errors. We have developed a hybrid functional pseudopotential generator, and present here the first rigorous investigation of pseudopotential density functional consistency for hybrid functionals. We provide benchmarking results of PBE0 pseudopotentials for the G2 dataset and some simple solids. Our results showed that the accuracy of geometric parameters compared to experiment improves when our new PBE0 pseudopotentials are used for PBE0 calculations. Also, the PBE0 pseudopotential has been implemented in OPIUM (http://opium.sourceforge.net).

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