Abstract Submitted
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Accurate and fast DFT calculations with the AM05 functional
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— The AM05 functional [1] has the same excellent performance for solids as the hybrid density functionals tested in Paier *et. al.* (J. Chem. Phys **124**, 154709 (2006); *ibid* **125**, 249901 (2006)). This confirms the original finding that AM05 performs exceptionally well for solids and surfaces. While hybrid functionals are computationally expensive, preveting them from being used in large systems and/or long molecular dynamics simulations, the AM05 functional is on a regular semi-local GGA form with corresponding computational cost. The performance of AM05 is even superior to an 'informed choice' between LDA and PBE. By comparing data from different electronic-structure codes we have determined that the numerical errors in this study are equal to or smaller than corresponding experimental uncertainties. Results for other systems will also be presented. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.
[1] R. Armiento and A. E. Mattsson, Phys. Rev. B **72**, 085108 (2005).

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