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Efficient band gap estimation for solids from DFT MARIA CHAN, GERBRAND CEDER, Massachusetts Institute of Technology — The ab initio prediction of band gaps for solids is important for fundamental and practical reasons. Unfortunately the most popular ab initio computation tool for solids, Density Functional Theory (DFT) in the Kohn-Sham implementation with local or semilocal exchange correlation functionals (LDA/GGA), suffers from the famous “band gap problem.” In Kohn-Sham DFT with LDA/GGA, the energy gaps between occupied and unoccupied single-particle states (Kohn-Sham gaps) are typically far below the experimentally-measured band gaps. In this talk we propose an efficient method for the estimation of fundamental band gaps in solids using DFT with local and semi-local functionals. We demonstrate significant improvements compared to Kohn-Sham band gaps on over 100 compounds with experimental band gaps between 0.5 and 4 eV (mean absolute error reduced from 0.84 to 0.25 eV, standard deviation from 0.5 to 0.2 eV). Our proposed method has an accuracy similar to the screened hybrid functionals and modified Becke-Johnson potentials, while requiring computational costs similar to typical DFT LDA/GGA calculations.

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