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Volume effects in band gap predictions for solids ANUBHAV JAIN, Massachusetts Institute of Technology, MARIA K. CHAN, Argonne National Laboratory, RICKARD ARMIENTO, GERBRAND CEDER, Massachusetts Institute of Technology — The *ab initio* prediction of band gaps for solids is important for fundamental and practical reasons. Many approaches exist to remedy the "band gap problem" in Density Functional Theory (DFT) in which band gaps are severely underestimated. We recently proposed the Δ-sol method [1], an adaptation of the ΔSCF method towards solids, in which the fundamental gap is evaluated using total energies from DFT. Using Δ-sol, we obtained band gaps for over 100 crystalline semiconductors at accuracies similar to those of hybrid functionals such as HSE, but at significantly smaller computational costs. However, the accuracy of band gap predictions from first principles remains dependent on accurate determination of lattice parameters and cell volumes. In this talk, we discuss the effects of the accuracy in lattice parameters on predicted band gaps. We present results on the accuracy of cell volumes determined using several exchange-correlation functionals: LDA, PBE, HSE and AM05, and compare the dependence of Kohn-Sham gaps and band gaps predicted using Δ-sol on cell volumes. Finally we discuss optimal approaches for predicting band gaps for compounds with unknown lattice parameters.

[1] M. K. Y. Chan and G. Ceder, Phys. Rev. Lett. 105, 196403 (2010)

Maria K. Chan
Argonne National Laboratory

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