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Relating the defect band gap and the density functional band gap[1] PETER SCHULTZ, Sandia National Laboratories, ARTHUR EDWARDS, AFRL/RVSE — Density functional theory (DFT) is an important tool to probe the physics of materials. The Kohn-Sham (KS) gap in DFT is typically (much) smaller than the observed band gap for materials in nature, the infamous "band gap problem." Accurate prediction of defect energy levels is often claimed to be a casualty—the band gap defines the energy scale for defect levels. By applying rigorous control of boundary conditions in size-converged supercell calculations, however, we compute defect levels in Si and GaAs with accuracies of $\sim$0.1 eV, across the full gap, unhampered by a band gap problem. Using GaAs as a theoretical laboratory, we show that the defect band gap—the span of computed defect levels—is insensitive to variations in the KS gap (with functional and pseudopotential), these KS gaps ranging from 0.1 to 1.1 eV. The defect gap matches the experimental 1.52 eV gap. The computed defect gaps for several other III-V, II-VI, I-VII, and other compounds also agree with the experimental gap, and show no correlation with the KS gap. Where, then, is the band gap problem? This talk presents these results, discusses why the defect gap and the KS gap are distinct, implying that current understanding of what the "band gap problem" means—and how to "fix" it—need to be rethought.

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