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Band gaps with approximate density functionals: the derivative discontinuity revealed from ensemble considerations ELI KRAISLER, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, Israel — The band gap is a central property of solids. Unfortunately, this quantity is not generally equal to the Kohn-Sham band gap of density functional theory (DFT), even in principle. The two band gaps differ precisely by the derivative discontinuity. Popular approximate functionals are thought to be devoid of a derivative discontinuity, thereby eliminating their usefulness for gap prediction. Here we show that all exchange-correlation functionals possess a derivative discontinuity, which arises naturally from the application of ensemble considerations within DFT. The approach requires no empiricism and involves no approximations beyond the choice of the exchange-correlation functional. Furthermore, the derivative discontinuity can be expressed in closed form using quantities obtained in the course of a standard DFT calculation of the neutral system, allowing for band gap calculations in periodic systems. The approach is demonstrated by calculations of the band gap for eleven representative insulators and semiconductors, using the ensemble approach with the local density approximation. We find that the derivative discontinuity revealed by this approach accounts for a significant part of the overall band gap and its inclusion reduces the error in band gap prediction from 50% to 10%.

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