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Failure of hybrid functionals to predict band gaps of materials at nanoscale XINQUAN WANG, ZHIGANG WU, Department of Physics, Colorado School of Mines — It is well known that density functional theory (DFT) within LDA/GGA severely underestimates band gaps in semiconductors and insulators due to the lack of derivative discontinuity in exchange-correlation, and hybrid functionals have been widely employed to improve band-gap calculations within the framework of DFT. In this work we show that hybrid functionals are not reliable in predicting band gap for nanostructures by comparing the hybrid functionals results of Si nanowires with those obtained using the many-body perturbation theory within the GW approximation. The hybrid functionals give a worse band-gap scaling law than that of LDA/GGA and their success in bulk materials is largely fortuitous, because they cannot correctly describe the response to the variation in screening.

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