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Exact-exchange density-functional calculations for large gap materials: A major step forward? RUDOLPH MAGYAR, Los Alamos National Laboratory, ANDRZEJ FLESZAR, Universitaet Wuerzburg , EBERHARD GROSS, Freie Universitaet Berlin — The electronic structure of several large gap insulators is calculated using the exact-exchange functional (EXX) in density functional theory, and the results are compared with those from the local-density approximation (LDA) and experiment. EXX is considered a major step beyond LDA and has already been shown to provide exceptionally accurate results for semi-conductors. In this study, two classes of large gap systems are examined, the noble-gas solids and simple biatomic ionic crystals. For the noble-gas solids, the dominant binding effect is the Van der Waals interaction which is not properly described by the EXX formalism. Ionic crystals, instead, are held together by the Hartree interaction between oppositely charged ions, and the Van der Waals interaction plays a negligible role. It is seen that the EXX method does not reproduce the fundamental energy gaps as well as has been reported for semiconductors; however, the EXX gaps are much closer to the optical gaps than LDA gaps and still represents a significant advance in band theory calculations.

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