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Role of screened exact exchange in accurately describing properties of transition metal oxides: Modeling defects in LaAlO₃

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Abstract

The properties of many intrinsic defects in the wide-band-gap semiconductor LaAlO₃ are studied using the screened hybrid functional of Heyd, Scuseria, and Ernzerhof (HSE) [J. Chem. Phys. 118, 8207 (2003)]. As in pristine structures, exact exchange included in the screened hybrid functional alleviates the band-gap underestimation problem, which is common to semilocal functionals; this allows accurate prediction of defect properties. We propose correction-free defect energy levels for bulk LaAlO₃ computed using HSE that might serve as a guide in the interpretation of photoluminescence experiments.

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