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Charge transition levels of oxygen vacancies in monoclinic hafnia[1]

MANISH JAIN, University of California at Berkeley and Lawrence Berkeley National Laboratory, JAMES R. CHELIKOWSKY, University of Texas at Austin, STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Laboratory — We perform electronic structure calculations on oxygen vacancies in hafnia using a combined density functional theory (DFT) and GW formalism. This formalism corrects for the error in calculating formation energy and charge transition levels using standard DFT. While the formalism is, in principle, exact; in previous calculations of this kind, one makes several approximations to make the calculation tractable. We assess the impact of these approximations on the charge transition levels of the oxygen vacancy in hafnia. In particular, we examine the assumption that the quasiparticle wavefunctions are the same as DFT wavefunctions for the defect states. We show that this assumption can lead to erroneous results in this system and present the charge transition levels without making use of this assumption. We also explore the possibility that these defects are negative U centers.

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