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Role of oxygen-related defects in hafnia[1] MANISH JAIN, Department of Physics, University of California, Berkeley and Lawrence Berkeley National Laboratory, JAMES R. CHELIKOWSKY, University of Texas, Austin, STEVEN G. LOUIE, Department of Physics, University of California, Berkeley and Lawrence Berkeley National Laboratory
— Hafnia has recently received much attention because of its potential application as high-k dielectric material replacing silica in microelectronic devices. Point defects in hafnia - in particular oxygen vacancies and interstitials - can play an important role as traps or sources of fixed charge. In this study, we perform electronic structure calculations on oxygen-related defects in monoclinic hafnia using a combined density functional theory (DFT) and GW formalism. We have previously shown that upon including quasiparticle defect levels and the appropriate electrostatic corrections within a supercell calculation, this formalism corrects for the error in calculating formation energy and charge transition levels using standard DFT. In this study, we calculate the formation energy of these defects as a function of the Fermi level and the chemical potential of oxygen to determine which of these defects are most stable.

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