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Optical behavior of native defects in ZnO[1] JOHN L. LYONS, DANIEL STEIAUF, AUDRIUS ALKAUSKAS, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — The behavior of native defects in ZnO has been fiercely debated for years, yet questions still remain regarding their fundamental properties. Once blamed for causing unintentional n-type conductivity, it is now well-established that native donors are highly unlikely to act as shallow donors in as-grown material. Still, both native donors and acceptors may be present in some samples, acting as either compensating acceptors or deep donors that may inhibit attempts to obtain high-conductivity n-type ZnO. In this work, we re-examine the properties of native donors and acceptors in ZnO using hybrid density functional calculations, which allow for the quantitative prediction of defect transition levels and formation energies. We focus on the optical and electrical properties of these defects, and calculate both their optical and thermodynamic transition levels. Most of the defects give rise to deep, broad luminescence signals that can serve as a means of experimentally verifying the nature of the center. We also examine how interactions with hydrogen interstitials affect the properties of these defects.

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