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First-Principles determination of deformation potentials and band parameters in group-II oxide semiconductors[1] QIMIN YAN, PATRICK RINKE, MATTHIAS SCHEFFLER, CHRIS G. VAN DE WALLE, Materials Department, UC Santa Barbara — Group-II oxide semiconductors (MgO, ZnO, and CdO) are excellent candidates for use in solid state lighting. Due to the lattice mismatch between oxide epilayers and substrates, strain effects (described by deformation potential parameters) play a crucial role in the band structure. On the other hand, the band dispersion in the vicinity of the band extrema (described by effective masses and Luttinger parameters) is also critical in determining the optical properties of the oxide-based materials and devices. We employ the Heyd-Scuseria-Ernzerhof (HSE) hybrid functional in density functional theory to overcome the limitations of local-density or generalized-gradient functionals (LDA and GGA) and produce highly accurate band structures. Using the k-p approach, we obtain consistent sets of band parameters (band gaps, crystal-field splittings, spin- orbit splittings, effective masses, and Luttinger parameters) for CdO, ZnO, and MgO in the wurtzite phase. We also report a comprehensive set of deformation potentials that describe band- structure modifications in the presence of strain. The results can be used for accurate modeling of device structures.

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