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Calculated polarizations and piezoelectric constants of wurtzite ZnO, CdO and MgO PRIYA GOPAL, UCSB — The macroscopic polarization in wurtzite crystal structures such as GaN and ZnO has a strong influence on the electrical and optical properties. This property has been exploited in GaN/AlGaN heterostructures, where the difference in the polarizations between layers induces an electric field at the interface forming a high mobility two-dimensional electron gas (2DEG) [1]. . Here we calculate the polarization and the piezoelectric properties of the corresponding wurtzite-structure binary oxides ZnO, MgO and CdO. The knowledge of these properties is essential to explore the possibility of creating similar high mobility polarization induced 2DEGs in the ZnO-based material system. However, since wurtzite-structure MgO and CdO are not experimentally accessible, the values can be obtained computationally. We use the recently developed self-interaction corrected pseudopotential (pseudo-SIC) implementation [2] of the density functional theory and the widely used Berry phase method [3] for obtaining the polarization and piezoelectric constants. We find that the polarization gradients between the end-point compounds in the MgO-ZnO-CdO are larger [4] than in the GaN analogues.

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