

Abstract Submitted
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Dependence of the band gap in the high-k dielectric HfO₂ on crystalline phase K. NISHITANI¹, P. RINKE, PH. EGGERT, S.J. HASHEMI-FAR, P. KRATZER, M. SCHEFFLER, Fritz-Haber-Institut der MPG — Recently HfO₂ has attracted considerable attention as a gate dielectric for (CMOS) CMOS technology, because it combines a wide band gap and good thermal stability with a low-frequency dielectric constant much higher than that of SiO₂. While the exact values of the band gap and band alignment with Si(001) are important for the application as gate dielectric, experimental data show some scatter possibly due to ill-defined crystallinity of the samples. We analyze the structural and electronic properties of both cubic and tetragonal HfO₂ employing density-functional theory within the local-density approximation (LDA) in a pseudopotentials, plane-wave approach. We find that cubic HfO₂ has a direct band gap, while the tetragonal phase exhibits a slightly larger indirect gap. Applying many-body perturbation theory in the *GW* approximation corrects the underestimation of the LDA band gap and gives band gaps within the experimentally reported range. We find that the energy shifts introduced by the *GW* self-energy are largely independent of the structure and show that the differences in band structure between the two phases arise mainly from internal relaxations of the oxygen atoms in the tetragonal phase, while the *c/a* value has little effect on the character of the band gap.

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