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Hybrid functional and quasiparticle calculations of the Schottky barrier height at TiN/HfO_2 interface YOUNG JUN OH, ALEX TAEKYUNG LEE, Department of Physics, KAIST, HYEON-KYUN NOH, Samsung Electronics Co., Ltd., K.J. CHANG, Department of Physics, KAIST — In high-k/metal gate transistors, it is important to control the metal work function such that it should be close to the valence and conduction band edges of Si in p- and n-channel devices, respectively. The Schottky barrier height (SBH) is affected by composition of metal gate, impurity, and deposition process. In theoretical studies, using the local density functional approximation, the SBH is severely underestimated because of the underestimation of the dielectric band gap. In this work, we perform both hybrid functional and quasiparticle calculations to improve the band gap and effective work function in TiN/HfO_2 interface. We consider two types of TiN/HfO_2 interface structures, which consist of either Ti-O or N-Hf interface bonds. Depending on the type of interface bonds, the SBH differs by 0.36 eV. In the many-body perturbation theory, the GW_0 approach, which employs the self-consistent Green's function and the full frequency-dependent dielectric function, greatly improves the agreement of the SBH with experiments. We discuss the effects of the self-consistency and the plasmon-pole approximation on the SBH. On the other hand, with the hybrid functional, the SBH is overestimated due to the larger downward shift of the valence band edge of HfO_2.

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