

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Density functional calculations of the Schottky barrier height and effective work function in Ni/oxide interfaces
HYEON-KYUN NOH, YOUNG JUN OH, ALEX TAEKYOUNG LEE, K.J. CHANG, Department of Physics, Korea Advanced Institute of Science and Technology — In high-k/metal gate stacks of complementary metal-oxide semiconductor devices, it is important to control the effective work functions of metals such that they should match to the doping levels of poly-Si gates. However, it is known that metal work functions are strongly affected by interface dipoles and defects. In this work, we perform first-principles density-functional calculations to study the Schottky barrier heights and the effective metal work functions in Ni/SiO₂ and Ni/HfO₂ interface structures. We use the advanced approaches such as hybrid density functional and quasi-particle *GW* calculations for the exchange-correlation potential and discuss the limitations of GGA calculations. We also examine the effects of O-vacancy defects introduced at the interface on the Schottky barrier height and the effective work function. We find that, in the Ni/HfO₂ interface, the *p*-type Schottky barrier height tends to increase with increasing of the defect density due to the charge transfer at the interface, whereas it is little affected in the Ni/SiO₂ interface.

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Date submitted: 26 Nov 2011

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