Abstract Submitted
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First principles analysis of the capacitance density of high-k nanocapacitors utilizing the orbital separation approach SHUSUKE KASAMATSU, Department of Materials Engineering, the University of Tokyo, SEUNGWU HAN, Department of Materials Science and Engineering, Seoul National University, SATOSHI WATANABE, Department of Materials Engineering, the University of Tokyo — In order to realize further scaling of electronic devices, capacitors and transistors with higher capacitance density are necessary. To this end, higher-k films of nanometer thickness are being considered for next-generation devices. However, high-k/metal interfaces often suffer from degraded dielectric properties due to, e.g., contamination, defects, and the intrinsic dead layer effect [1]. In this work, we developed a new first principles approach based on the Kohn-Sham formalism that we call orbital separation approach [2] to calculate the capacitance of nano-sized capacitors and examine the limit in capacitance density. In this method, the Kohn-Sham orbitals around the Fermi level of a metal/insulator/metal slab are separated into left and right electrode. The separated orbitals are occupied according to different Fermi levels to simulate the effect of bias voltage. We applied this approach to Au/MgO/Au and $SrRuO_3/SrTiO_3/SrRuO_3$ systems to examine the effect of the interface on the dielectric response. We confirmed that this method gives reasonable results. The impact of the intrinsic dead layer and that of defects on the capacitance are also examined.

[1] M. Stengel and N. Spaldin, Nature 443, 679 (2006).
[2] S. Kasamatsu et al., Phys. Rev. B 84, 085120 (2011).

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