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First-principles simulation of negative capacitance in a polydomain ferroelectric-paraelectric bilayer capacitor under bias SHUSUKE KASAMATSU, The Institute for Solid State Physics, the University of Tokyo, SATOSHI WATANABE, Department of Materials Engineering, the University of Tokyo, CHEOL SEONG HWANG, SEUNGWU HAN, Department of Materials Science and Engineering, Seoul National University — The use of negative capacitance materials is gaining attention in recent years as a path to achieving further scaling of nanoelectronic devices [1]. For example, it has been reported that the ferroelectric thin film in a ferroelectric (FE)-paraelectric (PE) bilayer capacitor exhibits negative capacitance, i.e., the bilayer capacitor has a higher capacitance than the capacitor with a single PE layer [2]. However, the mechanism for this effect, especially with regard to the dynamics of polarization domains under bias voltage, is poorly understood. To tackle this issue, we performed first-principles simulation of a metal/FE/PE/metal capacitor with 180° stripe domains under bias using our recently developed orbital-separation approach [3]. We find an antiferroelectric-like behavior with a polydomain-monodomain transition under 0.3 V. Capacitance boost (i.e., negative capacitance) is observed within the monodomain regime, and the transition itself is also found to be a source of capacitance enhancement. [1] G. Catalan et al., Nature Mater. 14, 137 (2015). [2] D. Appleby et al., Nano Lett. 14, 3864, (2014); A. I. Khan et al., Appl. Phys. Lett. 99, 113501 (2011). [3] S. Kasamatsu et al., Phys. Rev. B 84, 085120 (2011); Phys. Rev. B 92, 115124 (2015).

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