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Modeling of band alignment at the β-Ga_2O_3/β-$(Ga_{1-x}M_x)_2O_3$ interface (M=Al, In) STEFAN BADESCU, GREGG JESSEN, Air Force Research Laboratory, Dayton, OH — Beta gallium oxide (β-Ga_2O_3) is receiving a significant attention as a possible native substrate for electronic devices. The band alignment and electron accumulation at the interface between β-Ga_2O_3 and its alloys remains an open question. We describe our modeling of β-Ga_2O_3/β-$(Ga_{1-x}M_x)_2O_3$ (M=Al, In) interfaces based on the density functional theory. These are using the LDA+U method with large simulation cells with Hubbard U parameters extracted from accurate GW models. We find a range of compositions with relevant band shifts and a range of alloy epilayer thickness as a function of lattice mismatch.

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