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Controlled Confinement of Half-metallic 2D Electron Gas in $BaTiO_3/Ba_2FeReO_6/BaTiO_3$ Heterostructures: A First-principles Study¹ TANUSRI SAHA-DASGUPTA, S.N.Bose National Centre for Basic Sciences, Kolkata, SANTU BAIDYA, University of Duisburg-Essen, Duisburg, UMESH WAGHMARE, Jawaharlal Nehru Centre for Advanced Scientic Research, Jakkur, Bangalore, ARUN PARAMEKANTI, Canadian Institute for Advanced Research, Toronto, Ontario — Using density functional theory calculations, we establish that the half-metallicity of bulk Ba_2FeReO_6 survives down to 1 nm thickness in $BaTiO_3/Ba_2FeReO_6/BaTiO_3$ heterostructures grown along the (001) and (111) directions. The confinement of the two-dimensional (2D) electron gas in this quantum well structure arises from the suppressed hybridization between Re/Fe d states and unoccupied Ti d states, and it is further strengthened by polar fields for the (111) direction. This mechanism, distinct from the polar catastrophe, leads to an order of magnitude stronger confinement of the 2D electron gas than that at the $LaAlO_3/SrTiO_3$ interface. We further show low-energy bands of (111) heterostructure display nontrivial topological character. Our work opens up the possibility of realizing ultra-thin spintronic devices.

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