Heterostructures of 3d-5d Double Perovskites: Potential Candidates for Confined Half-metallicity & High-T Quantum Anomalous Hall States

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Abstract

Considering the specific case of double perovskite (DP) compound Ba_2FeReO_6 (BFRO) made out of 3d transition metal (TM) ion Fe and 5d transition metal ion Re, we show that by embedding the BFRO in the band insulator $BaTiO_3$ (BTO) in a heterostructure quantum well geometry, the electrons of the DP can be confined to two dimensions due to potential energy mismatch created between the TM ions in the DP and in the insulating oxide. The 2D confinement achieved in the BTO/BFRO/BTO quantum well structures provides significant improvement over that in polar catastrophe-driven LAO/STO in terms of (i) 2D confinement length is an order of magnitude smaller, (ii) complete spin polarization of the 2D electron gas (2DEG), (iii) polarity control of the 2DEG, suggestive of magnetoelectric coupling, and (iv) realization of ultrathin half metals with topological bands.

Extending on the idea of driving topologically non-trivial features, we further find that BFRO/BTO geometry with termination at Fe layer, leads to formation of a C=1 quantum anomalous hall insulator (QAHI) state with a large topological gap ~100meV and an estimated FM T_c ~315K. The large gap and high T_c should enable practical use of our proposal. Our study identifies three key ingredients for the formation of this QAHI, which should be broadly applicable to other t_{2g} physics dominated 3*d*-5*d* or 3*d*-4*d* half-metallic DPs like Sr₂FeMoO₆ and Sr₂CrWO₆.

Work done in collaboration with Santu Baidya, Arun Paramekanti and Umesh Waghmare.

[1] Santu Baidya, Umesh V. Waghmare, Arun Paramekanti, and Tanusri Saha-Dasgupta, Phys. Rev. B **92**, 161106(R) (2015).

[2] Santu Baidya, Umesh V. Waghmare, Arun Paramekanti, and Tanusri Saha-Dasgupta, Phys. Rev. B **94**, 155405 (2016).