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First-Principles study of tris(8-hydroxyquinoline)iron(III) molecules: A promising spin filter material[1] WEI JIANG, MIAO ZHOU, ZHENG LIU, DALI SUN, Z. VALY VARDENY, FENG LIU, University of Utah, FENG LIU'S GROUP TEAM, Z. VALY. VARDENY'S GROUP TEAM — Using first-principles calculations, we have systematically investigated the structural, electronic, and magnetic properties of facial and meridional tris (8-hydroxyquinoline)iron(III) (Feq_3) molecules, solvent-free Feq_3 crystals and thin films. Our calculation results show that both Feq_3 isomers have a high spin state of 5 μ_B as the ground state when an on-site Hubbard-U term is included to treat the highly localized Fe $3d$ electrons, in agreement with experiment, while the standard DFT calculations produce a low spin Fe state of 1 μ_B. Furthermore, the freestanding Feq_3 films are found to be paramagnetic, but become Ferromagnetic (FM) within each layer when deposited on a NiFe substrate. This is induced by a strong anti-ferromagnetic (AFM) coupling between the first molecular layer and FM substrate. Also, an AFM coupling is found between the molecular layers. These findings suggest that Feq_3 molecular films may serve as a promising spin filter material in spintronic devices.

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