Abstract Submitted
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Spinterface between tris(8-hydroxyquinoline)metal(III) molecules and magnetic surfaces: a first-principles study[1] W. JIANG, Univ of Utah, JINGYING WANG, DANIEL DOUGHERTY, North Carolina State University, FENG LIU, Univ of Utah, FENG LIU TEAM, DANIEL DOUGHERTY TEAM — Using first-principles calculations, we have systematically investigated the hybridization between tris(8-hydroxyquinoline)metal(III) (Mq_3, M = Fe, Cr, Al) molecules and magnetic substrates (Co and Cr). Mq_3 with different central metal elements but the same organic framework has dramatically different interaction with different magnetic substrates, which affect the interface state significantly. AFM coupling was observed between magnetic Mq_3 molecules and ferromagnetic (Co) as well as antiferromagnetic (Cr) substrate, manifested with a superexchange and direct exchange interaction, respectively. Such strong magnetic interfacial coupling may open a gap around the Fermi level and significantly change interface transport properties. Nonmagnetic Alq_3 molecule was found to enhance the interface spin polarization due to hybridization between the lowest unoccupied molecular orbitals (LUMO) of Alq_3 and metallic surface state. These findings will help better understand spinterface and shed new light on future application of Mq_3 molecules in spintronics devices.

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W. Jiang
Univ of Utah

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