Spinterface between tris(8-hydroxyquinoline)metal(III) molecules and magnetic surfaces: a first-principles study

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) (Mq₃, M = Fe, Cr, Al) molecules and magnetic substrates (Co and Cr). Mq₃ 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 Mq₃ 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 Alq₃ molecule was found to enhance the interface spin polarization due to hybridization between the lowest unoccupied molecular orbitals (LUMO) of Alq₃ and metallic surface state. These findings will help better understand spinterface and shed new light on future application of Mq₃ molecules in spintronics devices.

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