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Transport properties of two-dimensional metal-phthalocyanine junctions: An ab initio study¹ SHUANG-LONG LIU, YUN-PENG WANG, XIANG-GUO LI, HAI-PING CHENG, University of Florida — We study two dimensional (2D) electronic/spintronic junctions made of metal-organic frameworks via first-principles simulation. The system consists of two Mn-phthalocyanine leads and a Ni-phthalocyanine center. A 2D Mn phthalocyanine sheet is ferromagnetic half metal and a 2D Ni phthalocyanine sheet is nonmagnetic semiconductor. Our results show that this system has a large tunnel magnetic resistance. The transmission coefficient at Fermi energy decays exponentially with the length of the central region which is not surprising. However, the transmission of the junction can be tuned using gate voltage by up to two orders of magnitude. The origin of the change lies in the mode matching between the lead and the center electronic states. Moreover, the threshold gate voltage varies with the length of the center region which provides a way of engineering the transport properties. Finally, we combine non-equilibrium Greens function and Boltzmann transport equation to compute conductance of the junction.

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Shuang-Long Liu
University of Florida

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