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Magnetism and spin transport in transition metal organometallic clusters

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Transition metal organometallics has recently attracted much attention due to its potential for applications in catalysis, molecular recognition, high-density storage, quantum computing, and spintronics. Despite these applications, reliable theoretical and experimental knowledge of energetics, dissociation energy, spin multiplicity, spin gaps, etc. of these systems is still missing. Therefore, we have performed very accurate fixed-node quantum Monte Carlo (QMC) calculations with the quest to elucidate electronic, magnetic, and atomic structure of these systems in both neutral and charged states and thus to provide ultimate answers to the open questions. For half-sandwich systems (vanadium-benzene and cobalt-benzene) which are important model systems for magnetic adatoms on graphene, we find results qualitatively different from DFT predictions for both spin ground-states as well as for fragmentation energies. Perhaps surprisingly, we conclude that also some experimental results may be strongly biased. We have also studied full-sandwich vanadium-benzene multi-decker clusters, V_nBz_{n+1}, n=1-3 in both neutral and charged states. The most important prospective applications of these and related systems are in spintronics as spin filters. Use as spin filters requires them to be half-metal ferromagnets, in order to feature a metallic gap for the minority-spin electrons and semiconducting gap for the majority-spin electrons. We find that, while magnetic structure of these systems is consistent with ferromagnetic coupling, their electronic structure is not consistent with half-metallic behavior as previously assumed, but rather these systems are ferromagnetic insulators with large and broadly similar ↑-/↓-spin gaps, implying thus a limited potential of these and related materials for spintronics applications unless they are further modified or functionalized.

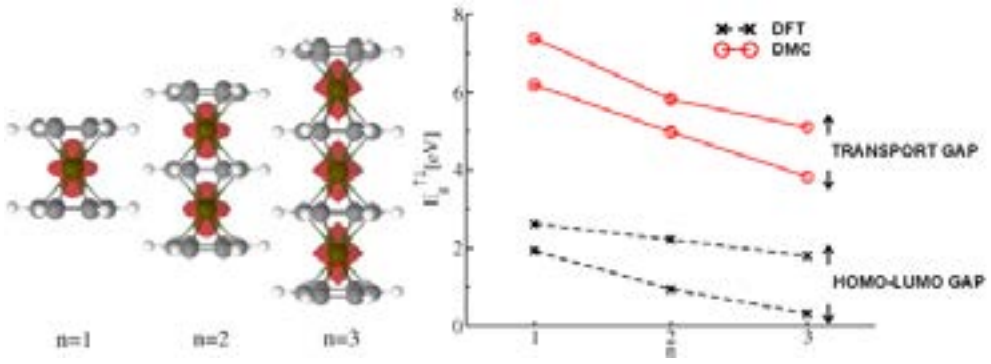

Figure 1: Model of vanadium benzene full-sandwich molecules featuring ferromagnetically coupled vanadium atoms. Right: ↑-/↓-spin gaps for vanadium-benzene full sandwich structures in DFT and QMC treatments.

Biography

Ivan Štich has his current scientific interest in "Atomic-scale imaging and nano-manipulation with surface probe techniques, nano-tribology, and 2D materials and their functionalization". In addition to mean field electronic structure techniques, he also develops and applies ultra-accurate Quantum Monte Carlo methods for fermionic systems.

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