Abstract Submitted
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Quantum Monte Carlo Study of π-bonded Transition-metal Organometallic Sandwiches[1] IVAN STICH, LUCIA HORVATHOVA, MATUS DUBECKY, Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia, LUBOS MITAS, North Carolina State University, Department of Physics, Raleigh — Accurate quantum Monte Carlo (QMC) calculations enabled us to determine the structure, spin multiplicity, ionization energy, dissociation energy, and spin-dependent electronic gaps of neutral and positively charged vanadium-benzene and cobalt-benzene half-sandwich and sandwich systems. The most intriguing application of these systems is as spin filters. For this purpose we have used a multi-stage combination of techniques with consecutive elimination of systematic biases except for the fixed-node approximation in QMC. The-fixed node approximation was treated at different levels from quantum chemistry (CAS-SCF) to various DFT schemes such as GGA, meta-GGA, hybrid, double-hybrid and local-hybrid functionals. While QMC results indicate a very limited predictive power of mean field DFT methods for this class of systems, QMC results are quite stable with fixed-node approximation based on several classes of DFT orbitals. Our results significantly differ from the established picture based on previous less accurate calculations and point out the importance of high-level many-body methods for predictive calculations of similar transition metal-based organometallic systems.

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