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Ab initio **design of spin-filters using single organic molecules** NICOLAE ATODIRESEI, PREDRAG LAZIC, VASILE CACIUC, STEFAN BLÜGEL, Forschungszentrum Juelich, D-52425 Germany — The possibility of using the electron's spin in addition to its charge as information carrying physical quantity in future electronic devices has stimulated extensive experimental and theoretical studies over the last decade. The design of nanoscale spintronic elements in multifunctional devices relies on a clear understanding of the physics at electrode-molecule interfaces and in particular, the functionality of specific molecules in a given organic-metal surface environment. Using density functional theory simulations we have performed systematic studies on several organic molecules (e.g. benzene, cyclopentadiene radical and cyclooctatetraene) adsorbed on a ferromagnetic surface (e.g. 2ML Fe on W(110)). We show how the magnetic information can be transmitted through an interface formed even by a non-magnetic molecule adsorbed on the ferromagnetic metal surfaces. Furthermore, our calculations demonstrate that as for other aromatic molecules on metal surfaces [1], taking into account the van der Waals interaction is essential to precisely follow the charge transfer at the interface and the formation of spin- split molecule-metal hybrid states. Our results demonstrate that even in the case of non-magnetic molecules, a molecule-electrode system can act as an efficient molecular spin-filter if the electrode is magnetic. [1] N. Atodiresei et al. Phys. Rev. Lett. 102, (136809) (2009).

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