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Concepts and modelling tools in molecular spintronics

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Molecular spintronics is an emergent field combining the flexibility of molecular electronics and molecular magnetism with the advantages of spintronics. Its main goal is the manipulation of the eectron spin by a wise combination of *ad-hoc* molecules (magnetic or not) and inorganic substrate. Besides the rich magnetic behavior resulting from the interaction between a magnetic molecule and a metal surface, or vice versa, additional functions such as switchability by external parameters (light, voltage) can be integrated. Due to an almost infinite range of possible material combination, an extensive experimental investigation can evidently not be carried out. Therefore modelling approaches combined with driving physical concepts are necessary. In particular I will show that notions such as spinterface [1] and orbital engineering between the molecule and its substrate can efficiently be used to analyze and hopefully serve to devise strategies for the design of new materials or devices.
The presentation will be illustrated by a careful analysis of various relevant systems and their magnetotransport properties. I will first consider the case of nonmagnetic molecules in contact with a magnetic substrate. I will show how magnetic anisotropy can be tuned at a ferromagnetic/molecule interface [2], or how the adsorption geometry of a molecule affects its tunneling magnetoresistance [3] and based on orbital-symmetry arguments I will present molecular junctions that show perfect spin filtering [4]. Finally I will show recent results obtained with spin-crossover molecules forming well organized lattices on a gold surface while keeping their switching ability [5].

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[4] A. Smogunov and Y. Dappe, Nano Lett. **15**, 3552 (2015) – D. Li, Y.J. Dappe and A. Smogunov, Phys. Rev. B **93**, 201403(R) (2016).
[5] K. Bairagi et al, Nature Communication **7**, 12212 (2016).