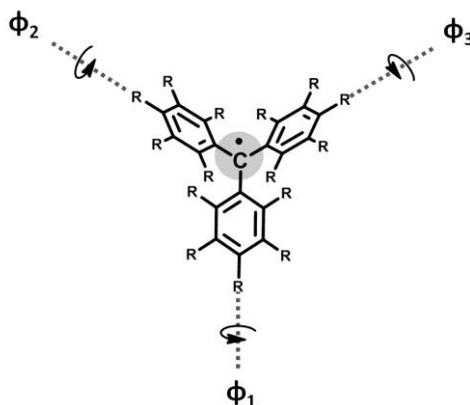


TRIARYLMETHYL RADICALS; TUNNABLE BUILDING BLOCKS FOR MOLECULAR SPINTRONICS

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Molecular Spintronics is a huge field that tries to take advantage of the electronic spin and charge in organic materials for the preparation of new devices^[1,2]. Within this field, π -aromatic molecular systems play an important role. They present high electronic conductivities comparing with their aliphatic analogues due to their π -conjugation^[3] which, in turn, is sensitive to the chemical and structural features of the system^[4]. Triarylmethyl radicals (TAMs) are very interesting in this respect^[5]. All TAMs are composed of three aryl rings bonded to a central carbon atom, where their unpaired electron mainly resides (see figure below). This family of π -aromatic radicals was the first to be discovered^[6], launching the field of organic radical chemistry in the early XXth century. Herein, we present a general relation between the spin localization in TAM radicals and a simple structural feature; the mean dihedral angle. We demonstrate the generality of this relation for different chemical functionalities and we test its stability at finite temperatures. In this way we highlight the potential of this simple spin/structure relation for future Spintronic applications under realistic conditions. Showing some examples of our designed 2D-materials based on this idea, we suggest that TAM radicals and their spin/structure relation could become a key-tool for the next step in molecular electronics.



- 1) Sanvito, S. *Nat. Mater.* **2007**, 6, 803–804.
- 2) Sanvito, S. *Chem. Soc. Rev.* **2011**, 40, 3336–3355.
- 3) Rocha, A. R.; García-Suárez, V. M.; Bailey, S. W.; Lambert, C. J.; Ferrer, J.; Sanvito, S. *Nat. Mater.* **2005**, 4, 335–339.
- 4) Venkataraman, L.; Klare, J. E.; Nuckolls, C.; Hybertsen, M. S.; Steigerwald, M. L. *Nature* **2006**, 442, 904–907.
- 5) Mas-Torrent, M.; Crivillers, N.; Mugnaini, V.; Ratera, I.; Rovira, C.; Veciana, J. *J. Mater. Chem.* **2009**, 19, 1691.
- 6) Gomberg, M. *J. Am. Chem. Soc.* **1900**, 22, 757–771.