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Proposition de titre:

Why and how to promote large spin/charge delocalization in molecule-based (magnetic) materials?

Proposition d'abstract:

Molecular engineering can be defined as the design of molecules or molecular assemblies whose architecture must enable to fulfill a function.[1] Historically developed for pharmaceutical sciences, this reasoned "bottom-up" approach is now applied into various fields such as photovoltaics, synthetic biology, energy or gas storage (batteries, MOFs…). It can operate at nanometric (molecules or molecular assemblies) and macroscopic scales (materials), and is taking advantage of the concepts and synthetic tools developed in molecular and supramolecular chemistries. This rational and elegant approach is also particularly attractive for the design of molecular architectures with preconceived and controlled magnetic and electronic properties.

After a general presentation of this approach and through the **experimental study** of a series of prototype dinuclear complexes (Figure),[2] we will see: i) what are the factors which govern the strength and sign of the magnetic exchange interaction through an aromatic ligand, and ii) how to promote electronic delocalization, a prerequisite for the **rational design of molecular conductors and/or magnets at high temperatures**. A couple of new room temperature molecule-based magnets and conductors made using this approach will then be discussed.[3]

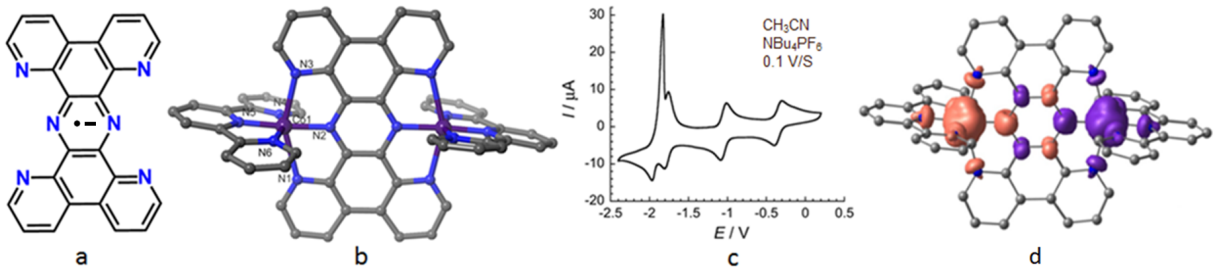

***Figure**. a) Tetrapyridophenazine (tphz$^{\bullet-}$) radical bridging ligand; b) Crystalline structure of the complex [Co_2(tphz$^{\bullet-}$)(terpyridine)$_2$]$^{3+}$; c) Cyclic voltammogram and d) spin density distribution in the same complex.*

References :

[1] Sillon B., *l'Actualité Chimique*, **2020**, *3*, 2.

[2] Ma, X., Suturina, E.A., Platunov, M., Rouzières, M., Wilhelm, F., Rogalev, A. Clérac, R., Dechambenoit, P., *J. Am. Chem. Soc.,* **2019***, 141*, 19, 7721; Ma, X., Suturina, E.A., De, S., Négrier, P., Rouzières, M., Clérac, R., Dechambenoit, P., *Angew. Chem. Int. Ed*. **2018**, 57, 7841.

[3] Perlepe P., Oyarzabal I., Mailman A., Yquel M., Platunov M., Dovgaliuk I., Rouzières M., Negrier P., Mondieig D., Suturina E. A., Dourges M.-A., Bonhommeau S., Musgrave R. A., Pedersen K. S., Chernyshov D., Wilhelm F., Rogalev A., Mathonière C., Clérac R., *Science,* **2020,** 370, 587 ; Suo M., Lou D., Yutronkie N., Clérac R., Dechambenoit P., *to be published soon.*