New results concerning Au- and Ni-bis(dithiolene) and -bis(diselenolene) conducting complexes

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Gold and nickel bis(dithiolene) and bis(diselenolene) complexes have provided conducting materials with unusual behavior. In this presentation we will report new results concerning the electronic structure of some of these conducting complexes both as neutral species and salts based on DFT calculations. The systems to be discussed are localized ambient pressure conductors either becoming metallic or keeping their activated conductivity under pressure [1-2]. The different (possible) roles of pressure in changing the conductivity regime will be discussed based on recent results for [Au-*R*,*R*-dm-dddt)$_2$] and [Ph_4P][Au(Me-thiazds)$_2$]$_2$. How the nature of intermolecular interactions and disorder can affect the conductivity variation of systems keeping the activated conductivity under pressure will be discussed on the basis of new results for Ni bis(dithiolene) and Ni bis(diselenolene) neutral complexes and salts.

References

[1] Y. Le Gal et al., *Journal of Materials Chemistry C* **9**, 12291-12302 (2021).
[2] A. Abhervé et al., *Journal of Materials Chemistry C* **9**, 4119-4140 (2021).