Title: **Organic-metal interfaces using DFT and GW ab initio methods**

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Abstract:
Large HPC calculations were used in the study of two very different phenomena concerning organic-metal interfaces. The first, the bright electroluminescence of individual GNRs suspended between the tip of a scanning tunneling microscope (STM) and a Au(111) substrate. Many body perturbation Theory calculations allowed the identification of the electronic states involved in the phenomena, localized at the GNR termini. The second is an advanced organic spin-interface architecture with magnetic remanence at room temperature. Density Functional Theory calculations shows how antiferromagnetic and/or ferromagnetic coupling can be optimized by selecting the molecular orbital symmetry.

[1] Chong, M. C., Afshar-Imani, N., Scheurer, F., Cardoso, C., Ferretti, A., Prezzi, D., & Schull, G. (2018). Bright electroluminescence from single graphene nanoribbon junctions. *Nano letters*, *18*(1), 175-181.
[2] Avvisati, G., Cardoso, C., Varsano, D., Ferretti, A., Gargiani, P., & Betti, M. G. (2018). Ferromagnetic and antiferromagnetic coupling of spin molecular interfaces with high thermal stability. *Nano letters*, *18*(4), 2268-2273.