Tuning Spin States in Graphene Nanoribbons via Metal Spin Centres and Chemical Coupling

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Graphene nanoribbons (GNRs) can be synthesized with atomic precision, offering a versatile platform for exploring novel electronic and chemical properties[1]. The integration of porphyrin units into GNR structures enables the periodic incorporation of transition metal ions, opening pathways for tunable electronic, magnetic, and catalytic functionalities. However, the synthesis and characterization of such hybrid systems remain challenging due to their complexity and high cost[3,4]. To address this, theoretical calculations serve as essential complementary tools for the design and optimization of transition metal-functionalized GNRs. In this work, I developed a computational workflow for studying hybrid GNR-porphyrin-metal systems, utilizing various ab initio methods to investigate their structural, electronic, and magnetic properties. A series of transition metals, including 3d metals and lanthanides, are incorporated into the study to explore their effects on the material's properties. Additionally, different chemical couplings between GNRs and porphyrins are highlighted, offering insights into their influence on the functionality of these materials. This approach provides valuable insights for guiding experimental efforts and advancing the development of functionalized GNR-based materials.

References

1. Cai et al, Nature 466, 2010, 470-473
2. Gu et al, Angewandte Chemie 137, 2025, e202417129
3. Chen et al, Nature Chemistry 16, 2024, 1133-1140

Figures

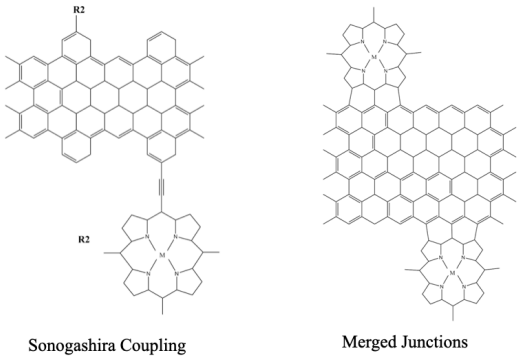

Figure 1: Chemical structures of the GNR-porphyrin-metal systems studied, featuring incorporated divalent 3d transition metals and trivalent lanthanides.