Electronic and Magnetic Properties of Organic Kagome Polymers

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Abstract:

Recent studies on carbon-based triangulene (CTN) dimers and hexamer nanostars on Au(111) surface have revealed that high spin states of adsorbed species are not totally screened by the metal and that magnetism may persist [1-2]. Based on first-principles density functional theory (DFT), we propose a promising route to control the quantum phase transition in 2D organic polymers based on CTN monomers by incorporating lightweight elements like boron or nitrogen [3-4]. Although the pure triangulene based Kagome polymer shows Mott-insulating antiferromagnetic phase, inducing organic substituants like B and N can alter the magnetic phase to ferromagnetic. Moreover, the symmetry in these types of polymers play a major role on the electronic structure, specially in controlling the band dispersion around Fermi level. Furthermore, a longer linker between the monomers can amplify the total magnetic moment along with the topological edge states. In addition, B-substituted polymers exhibit high mobility carriers while the N-substituted polymers are half-metallic where the minority spin shows mobility close to silicon. In brief, this presentation will mainly focus on different aspects to uncover collective magnetism in metal-free nanosystems. These findings may open the door for various low-dimensional organic nanomaterials based new quantum phenomena to achieve room-temperature superconductivity for applications in eco-friendly biodegradable solid-state spintronic devices.

References

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Figures

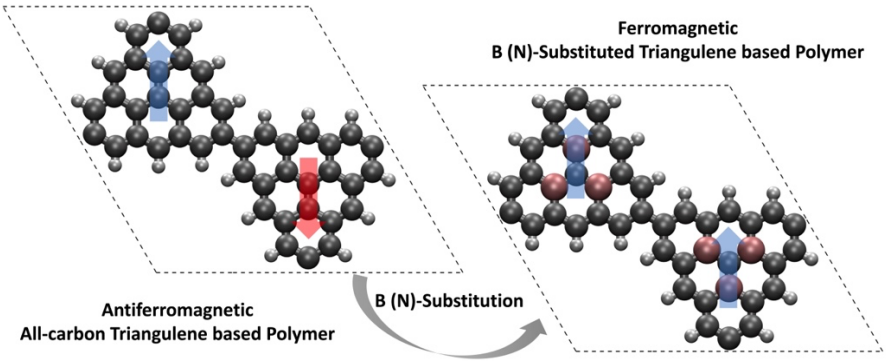

Figure 1: Tuning the magnetic phase of carbon derived Kagome polymers by B(N) substitution.