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Long-range magnetic order in metal-free two-dimensional materials

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Magnetism is typically connected with metal atoms, and long-range magnetic ordering with spin-orbit coupling. We present a new concept to generate strong ferro- and antiferromagnetic coupling in metal-free materials based on radical polyaromatic building blocks such as heterotriangulenes, which are arranged in regular planar honeycomb-kagome lattices.
We will share our theoretical considerations for the design of metal-free magnetism in 2D systems. Following basic considerations (Lieb theorem or Ovchinnikov rule), systems made of pure carbon lattices such as coupled triangulenes will give antiferromagnetic ground states. We will present two routes to achieve strong ferromagnetic couplings. In the first one, we will utilize heterotriangulanes. Due to the presence of foreign atoms, the Ovchinnikov rule is violated and ferromagnetic coupling is possible. We observed cases with coupling constants above 50 meV. A second route is to construct heterostructured lattices made of two different building units, so that the spins reside in the same graphene-like sublattice and the Ovchinnikov rule holds. We will present systems with Curie temperatures above 500K.
Finally, we present a strategy for the stabilization and synthesis of metal-free magnetic systems based on a switching strategy between zwitterion and biradical.

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