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Ultrafast Spin Dynamics in Magnetic-Atom-Doped Triangulene Nanoflakes

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ABSTRACT

The development of novel spintronic devices based on spin manipulation in magnetic nanostructures is crucial for achieving higher speed and miniaturization in future computing technologies. As a unique type of graphene quantum dot, triangulene nanoflakes (TNFs) exhibit nontrivial magnetic properties and excellent extensibility, making them highly promising for the design and application of spin logic units. In this study, we employ first-principles calculations to investigate experimentally synthesizable TNFs, in which transition metal (TM) atoms — namely Fe, Co, Ni, and Cu— are individually introduced at π-conjugated doping sites. The effects of different dopants and doping positions on the atomic configurations, electronic structure, and spin dynamics of the system are fully examined. The results reveal that the planar structure of TNFs remains stable upon the doping of magnetic atoms, while their intrinsic magnetism interacts intriguingly with the doped TM atoms. Notably, under specific doping conditions, a binary spin density distribution emerges, opening up possibilities for complex spin-dynamic scenarios beyond the spin flip. In this work, the spin-transfer processes, which typically required the participation of at least two magnetic centers in previous studies, can also be achieved in such single-magnetic-center-decorated systems. Interestingly, regardless of the initial spin direction, reversible spin-transfer processes can be realized using the same laser pulse. Expanding the pool of elementary processes to include not only spin-direction-dependent but also spin-direction-independent scenarios enables more versatile spin-logic operations, including both classical information processing and quantum computing. Building upon this, we further investigate the size effect of TNFs on the spin density distribution. The findings shed light on the design of spintronic device units based on TNFs. Finally, inspired by the concept of material extension for logical function integration, we explore spin transport in TNF dimers and propose a follow-up study on strain modulation. These findings pave the way for the practical implementation of nanoscale spintronic devices.

KEYWORDS

Magnetic nanostructures; triangulene; ultrafast spin dynamics; first principal calculations

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