Topological Design of Low-Dimensional Carbon Materials for Novel Spintronics

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Low-dimensional carbon allotropes (0D to 2D) exhibit intriguing geometry-dependent electronic and magnetic properties, making them promising candidates for spintronic applications. In this talk, we present our theoretical investigations on all-carbon materials, focusing on their spin separation, combination mechanisms, and band structure modulations. We explore the chemical tuning of spin states through rational molecular design, beginning with zero-dimensional triangulene fragments and their spin combination rules under various connectivity schemes and size amplifications. Extending these concepts, we investigate how superatomic assemblies can form one- and two-dimensional periodic structures, such as magnetic covalent organic frameworks, and analyze their impact on spin-polarized band structures. Furthermore, we introduce our theoretical framework on topological effects in one-dimensional nanoribbons and chiral carbon nanotubes, revealing new possibilities for spin control. Through these studies, we establish design principles for carbon-based spin interactions and assess their potential for next-generation spintronic materials.

References

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