Spin Polarisation In Large-Angle Twisted Bilayer Graphene On Nickel Substrate

Dana R. Engelgardt[1], Artem V. Kuklin[2], Pavel V. Avramov[1]
[1]Department of Chemistry, College of Natural Sciences, Kyungpook National University, (41566) 80 Daehak-ro, Buk-gu, Daegu, South Korea
[2]Department of Physics and Astronomy, Uppsala University, Box 516, SE-751 20 Uppsala, Sweden

qchemist@knu.ac.kr

The exploration of twisted bilayer graphene (tBLG) on Nickel (Ni) substrate presents a groundbreaking avenue for investigating novel physicochemical phenomena driven by the interplay of graphene's electronic properties and magnetic substrates. Twisted bilayer graphene, characterized by a mismatch angle between two stacked graphene layers, has a specific pattern called Moiré interference pattern caused by mismatch between graphene sheets (Fig. 1). The unique super-lattice structure introduces van Hove singularities (VHS) in the electronic density of states (DOS) and activates phonons within the graphene Brillouin zone [1]. While extensive research has been conducted on the interfaces between graphene and late transition metals [2], the potential interfaces involving tBLG remain largely unexplored.

In this study, tBLG on Nickel substrate (Fig. 1) structures with different rotation angles were designed and calculated. Here we want to demonstrate how spin related properties in tBLG, induced by magnetic substrate, could be varied depending on rotation angle between two graphene layers (Fig. 2). Spin-polarized calculations were performed within density functional theory (DFT) with the Perdew-Burke-Erzenhof (PBE) exchange-correlation functional and Periodic Boundary Conditions (PBC) to describe the electronic structure and induced magnetic properties in tBLG.

Artificial intelligence (AI) significantly enhances the analysis and optimization of these complex objects due to their large structures which are hard to calculate using first principles methods. Again, machine learning can process large datasets from DFT calculation to identify correlations between rotation angles and electronic structure. Also, these algorithms can predict the behavior of tBLG under various conditions (external magnetic of electric field etc.), facilitating the discovery of optimal configurations for specific applications. The integration of AI in the analysis of tBLG on magnetic substrates represents a significant step forward in the quest for high-performance, multifunctional materials.

References

[1] Jorio A., Cançado L.G., Solid State Communications, 3-12 (2013) 175-176
[2] Ivan S. Sokolov, Dmitry V. Averyanov, Oleg E. Parfenov, Igor A. Karateev, Alexander N. Taldenkov, Andrey M. Tokmachev, and Vyacheslav G. Storchak, Materials Horizons, 7 (2020), 1372-1378

Figures

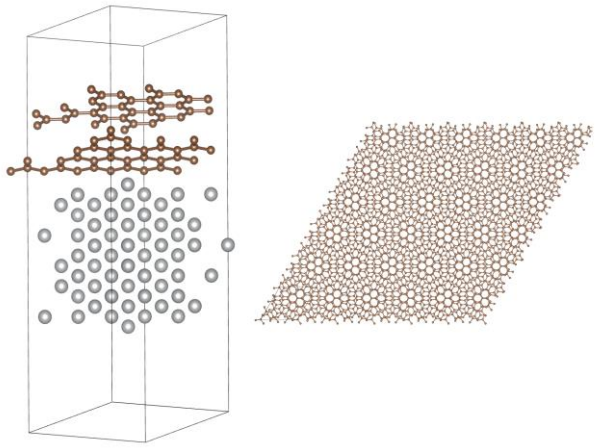

Figure 1. Left panel: structural model of twisted bilayer graphene on a nickel substrate, carbon atoms are depicted in brown, nickel in gray; right panel: Moire pattern in the twisted bilayer graphene system (top view)

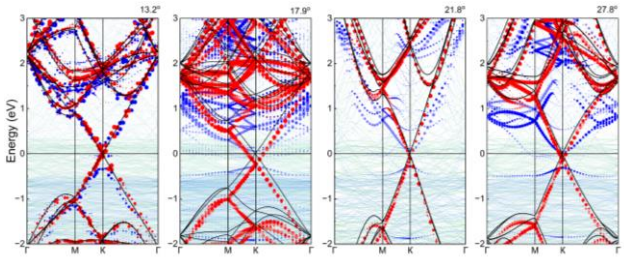

Figure 2. Band structures (BS) of twisted bilayer graphene on a nickel substrate with different rotational angles. Red lines represent spin-up states, blue lines denote spin-down states, and black lines show the BS of twisted bilayer graphene structures without the substrate for comparison