SPIN POLARISATION IN LARGE-ANGLE TWISTED BILAYER GRAPHENE ON NICKEL SUBSTRATE

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This is of advanced area related to new physicochemical phenomena in twisted bilayer graphene. Twisted bilayer graphene (tBLG) is bigraphene system with a mismatch angle between two hexagonal structures. The interference between the two rotated layers generates a super-lattice with an angle-dependent wavevector that gives rise to van Hove singularities (VHS) in the electronic density of states (DOS) and activates phonons in the interior of graphene Brillouin zone [1]. The interfaces between graphene and late transition metals have been thoroughly studied in recent years [2] but researchers haven't paid their attention to possible interfaces with twisted bilayer graphene. TBLG on Nickel substrate (Fig. 1, a) 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 changed depending on rotation angle between two graphene layers (Fig.1, b). 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.

References

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[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

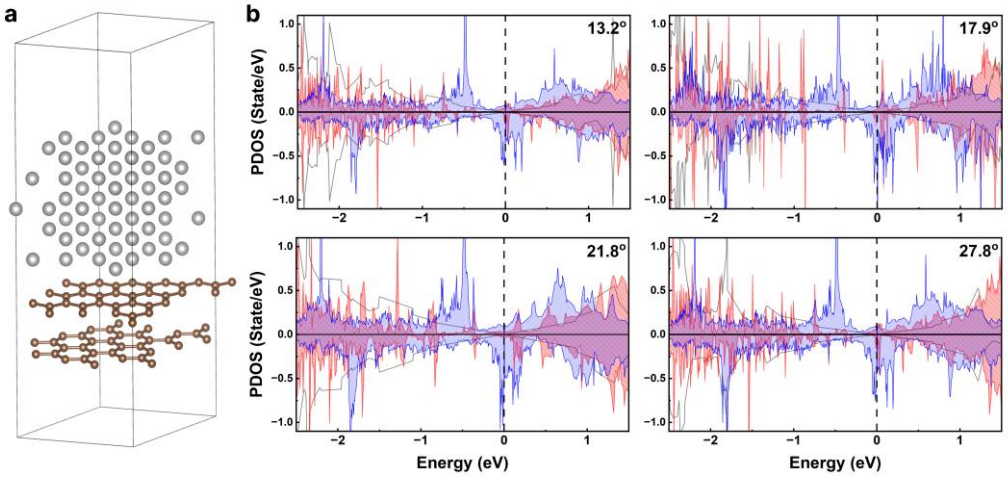

Figure 1: a. twisted bilayer graphene on Ni substrate model; b. partial density of states (PDOS) for the different rotation angle in first (blue) and second (red) layer of graphene in tBLG on Ni substrate, DOS of tBLG without substrate is a grey line