Magnetic effects emergence in doped-twisted bilayer boron nitride

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Twisted stacking of two-dimensional systems has emerged as a new platform for studying novel quantum phenomena, such as the strongly correlated states and superconductivity observed in twisted bilayer graphene at the magic angle. Building on these insights, exploring other twisted bilayers could unveil a broader spectrum of new physics and applications, potentially revolutionizing the semiconductors field. Specifically, band structure engineering—controlled by the interlayer rotation angle between bilayers—enables us to tune the fundamental properties of materials and investigate new phases of matter, including those associated with magnetic phenomena. In the case of twisted bilayer boron nitride (TBBN), the interlayer rotation angle induces flat bands without magic angles. Our first-principles calculations demonstrate that hole doping in the presence of these flat bands leads to the emergence of a magnetic phase, which strongly depends on the twist angle. As the twist angle decreases, a localized state appears at the top of the valence band, changing the density of charges needed to induce the magnetic phase. We discuss in detail the nature of these localized states and their implications for the electronic and magnetic properties. Additionally, we found that this magnetic phase exhibits intriguing characteristics, such as enhanced spin polarization, which could inspire new trends in spintronics research.