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Magic with Stacked 2D Semiconductors

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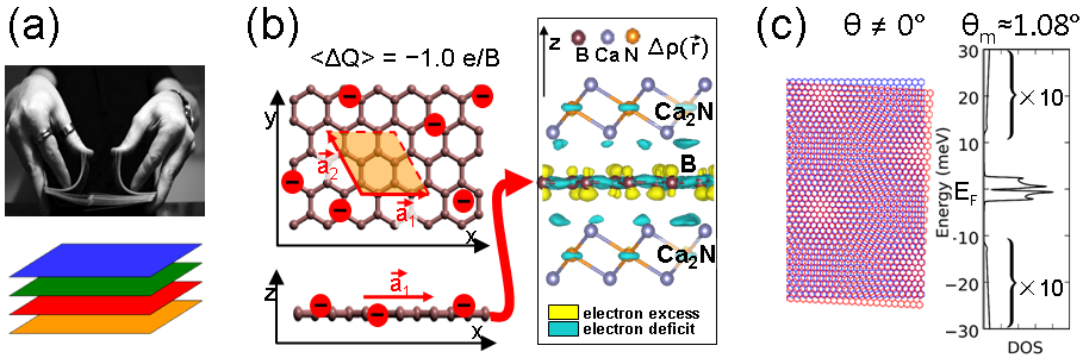

Figure 1: (a) Card magic illustrating the van der Waals assembly of 2D materials to a functional nanostructure. (b) Conversion of a 2D boron monolayer to a honeycomb lattice due to electron doping provided by a 2D electride. (c) Unusual changes in the electronic structure of twisted bilayer graphene near the magic twist angle $\theta_m \approx 1.08°$.

Like in a magic trick, atomically thin layers of specific materials can be mixed and stacked in a well-defined way. Due to the inter-layer interaction and charge transfer, the heterostructure may exhibit sometimes unexpected behavior. This occurs in the case of elemental boron, which is notorious for a large number of stable allotropes not only in 3D bulk, but also in 2D. We find that a previously unknown 2D ε–B allotrope converts stepwise to a stable honeycomb structure when doped with electrons, resembling a magic conversion of boron to carbon atoms that carry one more valence electron [1]. As seen in Fig. 1(b), sufficient extra charge to initiate this transition may be provided when 2D boron is brought into contact with the 2D electride Ca_2N. A different apparent example of magic involves the previously overlooked twist degree of freedom in 2D structures like bilayer graphene, which changes the Moiré pattern, as shown in the left panel of Fig. 1(c). Recent theoretical and experimental evidence suggests that the electronic structure near the Fermi level of twisted bilayer graphene (TBLG) depends extremely sensitively on the twist angle θ. Near the magic angle value $\theta_m \approx 1.08°$, a flat band emerges at E_F, separated from conduction and valence states by energy gaps. This unexpected behaviour likely provides valuable insight into electron correlation and superconductivity in 2D systems. Even though TBLG and related non-periodic structures can not be treated by standard band structure theory, their electronic structure can be interpreted quantitatively using a parameterized model [2] that can be simply extended to consider also other deformations including shear [3].

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References

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