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MAGIC OF CARBON ON THE NANOSCALE

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With its complex behavior, which is becoming unveiled by *ab initio* DFT calculations, carbon fills a unique place in the periodic table. Both graphene and related nanometer-wide carbon nanotubes (CNTs) are unusually stable both mechanically and thermally. A structure consisting of graphite oxide, a fleece of CNTs, and strong carbon fabric layers may become the long-sought magic membrane capable of filtering and desalinating water [1] without the shortcoming of commercial reverse osmosis membranes. CNTs may also be used as magic autoclaves and nanoreactors capable of transforming enclosed $NbCl_3$ molecules Nb metal [2]. The concerted transformation process is accelerated by the catalytic activity of the CNT that lowers activation barriers and the conversion temperature to below the high melting temperature T_M=2,750 K of Nb. A third example of apparent magic involves the twist degree of freedom in layered 2D structures, which changes the Moiré pattern shown in Fig. 1. Recent evidence suggests that the twisted bilayer graphene (TBLG) develops a flat band near the magic twist angle $\theta_m \approx 1.08°$, which is separated by gaps from conduction and valence states. This behavior can not be studied by standard band structure theory methods, but parameterized models allow quantitative description of electronic structure changes [3] including their dependence on shear [3].

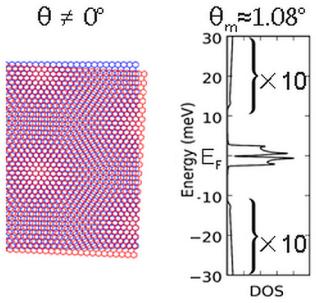

Figure 1. Unusual changes in the electronic structure of twisted bilayer graphene near the magic twist angle $\theta_m \approx 1.08°$.

References

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