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Using Hidden Degrees of Freedom in 2D Materials

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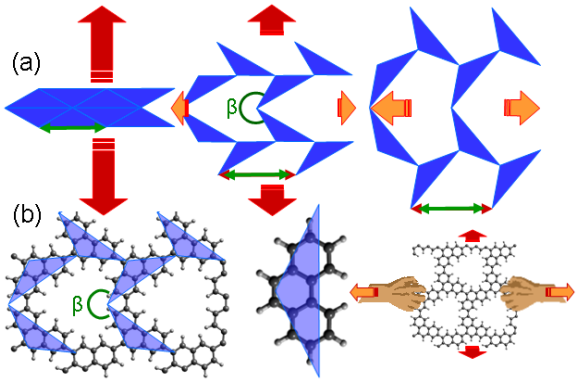

Figure 1
(a) Global deformation in a kirigami lattice of linked triangles.
(b) Porous graphene as nanometer-sized counterpart of a kirigami lattice of polymerized phenanthrene molecules. (Ref. [2]).

Rising interest in using auxetic materials with a negative Poisson ratio as smart structural components in macro-scale architecture [1] is providing inspiration in the realm of 2D nanostructures. An assembly of rigid isosceles triangles hinged at their corners on the macroscale or polymerized phenanthrene molecules forming porous graphene on the nanoscale, shown in Fig. 1, is a mechanical metamaterial with macro-scale properties differing fundamentally from those of its microscopic components [2]. Curiously, not only the length-to-width aspect ratio of the entire system, but also its Poisson ratio depends sensitively on a hidden variable, the closing angle β, resulting in a shape-memory effect. In this and in a large class of related structures, which can be deformed by uniaxial strain at low energy cost, the Poisson ratio may change sign and even diverge for specific values of β. On the nanoscale, deformations change the interaction between constituent nanostructures, behaving as quantum dots, and thus the electronic and optical properties of the entire system. A different hidden degree of freedom, which had been ignored for a long time, is the twist angle θ between layers in a bilayer of graphene or other 2D substances. In twisted bilayer graphene (TBLG), the electronic structure near the Fermi level depends sensitively on θ. Emergence of a flat band, separated from the conduction and the valence states by energy gaps, had been predicted and observed near the magic angle value θ_m =1.1°, providing new insight into electron correlation and superconductivity in 2D systems. Even though TBLG and related non-periodic structures can not be treated by band structure theory, their electronic structure can be interpreted quantitatively using a parameterized model [3] that can be simply extended to consider also other deformations including shear [4].

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References:

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[4] Xianqing Lin, Dan Liu and David Tománek, *Shear instability in twisted bilayer graphene,* Phys. Rev. B. ***98,*** 195432 (2018).