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The Mechanical properties of graphene-derived materials:

A multiscale model studies

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Graphene-based papers attract particular interests recently owing to their outstanding properties, the key of which is their layer-by-layer hierarchical structures similar to the biomaterials such as bone, teeth and nacre, combining intralayer strong sp2 bonds and interlayer crosslinks for efficient load transfer. Here we firstly study the mechanical properties of various interlayer and intralayer crosslinks via first-principles calculations and then perform continuum model analysis for the overall mechanical properties of graphene-based papers. We proposed here a deformable tension-shear (DTS) model by considering the elastic deformation of the graphene sheets, also the interlayer and intralayer crosslinks. The DTS is then applied to predict the mechanics of graphene-based paper materials under tensile loading.
We propose a strengthening and toughening model multimodal and self-healable crosslinks, consisting of long, strong and short, self-healable ones, to enhance the mechanical properties of graphene-drived materials. The results show that with the brick-and-motar hierarchy of these materials, multimodal crosslinks synergistically transfer the tensile load to enhance the strength, whereas fracturing and reforming of the reversible crosslinks improve the toughness significantly. The findings here could shed light on the development of high-performance paper-, fiber- or film-like macroscopic materials from monolayer nanosheets with nanoengineerable interfaces.

Keywords: Graphene-derived materials, Deformable tension-shear (DTS) model, crosslink, self-healing,