Tailoring Mechanical and Thermal Properties of Graphene Origami

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Abstract: Origami approach, an art of folding paper, is used to generate three-dimensional complex structures for extraordinary properties. However, the generation of graphene origami is still challenging. Here, using molecular dynamics simulations and density functional theory calculations, we show that patten-based hydrogenation (Figure 1a) can be employed to generate a wide range of complex graphene origami. Our results show that graphene Miura origami (Figures 1b and 1c) can show excellent properties, such as super compressibility and stretchability, negative Poisson's ratio behaviour (Figure 1b), and highly tunable coefficient of negative thermal expansion (Figure 1d). The super compressibility and stretchability and negative Poisson's ratio behaviors is due to the Miura origami geometry (extrinsic property). On the other hand, the negative coefficient of thermal expansion is due to inseparable combination of the pattern-based hydrogenation, Miura origami geometry, and large out-of-plane thermal fluctuations (intrinsic property of graphene). This study also opens opportunities to obtain other multi-functional materials by combination of hydrogenation, intrinsic properties of graphene, and three-dimensional geometry.

References

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Figures

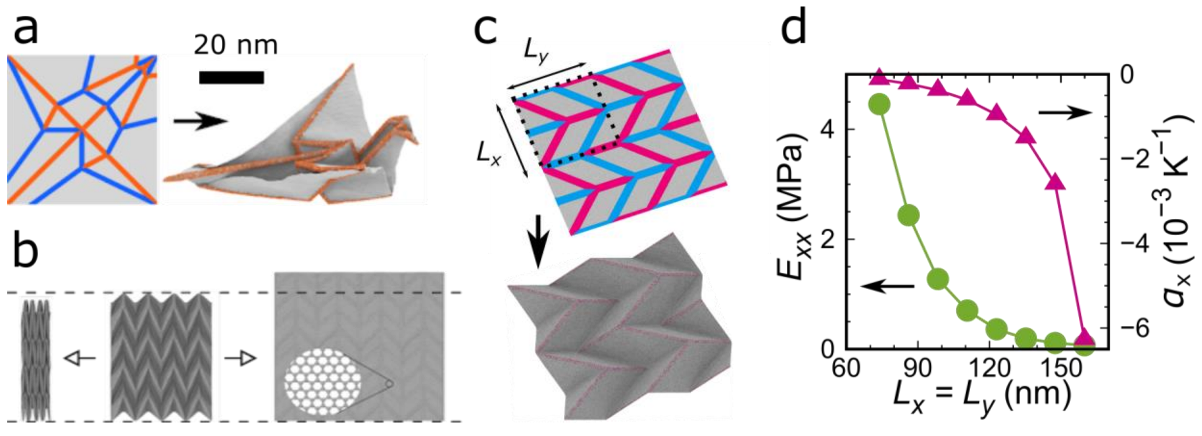

Figure 1. (a) Patten-based hydrogenation for the formation of a graphene flapping bird origami. Hydrogenation is conducted on the top of graphene in the areas coloured in red and on the bottom of graphene on the area coloured in blue. (b) Super compressibility and stretchability and negative Poisson's ratio behaviour of a graphene Miura origami structure. (c) The pattern-based hydrogenation of a Miura graphene origami. (d) Coefficient of thermal expansion α_x and Young's modulus E_{xx} as functions of $L_x = L_y$ defined in (c).