Supplementary Information

Negative Poisson’s Ratio in 2D Life-boat Structured Crystals

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The calculation about the rotation and stretch of the bonds

The bond rotation and stretch happen simultaneously in a strain-engineered process. To estimate the energy change dominated by only rotation or stretch effect, a rigid approach can be used by fixing the other variables but relaxing those expressing the rotation or stretch. To compare the $\frac{\partial U}{\partial r}$ and $\frac{\partial U}{\partial \theta}$, the limit definition of partial derivative can be used:

$$\frac{\partial U}{\partial r} = \lim_{\Delta r \to 0} \frac{\Delta U}{\Delta r}(\theta, \phi)$$

$$\frac{1 \partial U}{r \partial \theta} = \frac{1}{\lim_{r \Delta \theta \to 0} \Delta \theta}(r, \phi)$$

The ratio of $\frac{\partial U}{\partial r}$ in $\delta$-phosphorene, $\delta$-arsenic and $\delta$-graphene under strain in the armchair direction are approximately 5:1, 2.2:1, and 1.2:1, respectively.

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