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Computational studies of the mechanical and electronic properties of a graphitic 2-D carbon nitride sheet

Two dimensional (2-D) sheet of graphitic carbon monolayer exhibit the astounding physical properties, as well as very promising applications in various field [1]. Recently, another 2-D family known as graphitic porous carbon nitride (CN) sheets have gained special interest due to their unique potentials in photochemical water splitting and as membrane for separation of gases [2,3]. The two most stable CN allotropes are heptazine and s-triazine sheets. As can be seen in Figure 1, the heptazine sheet hexagonal rings are arranged in abreast manner whereas s-triazine sheet has two of its hexagonal rings separated through C-C bond. Because of the wide range of the CN sheets applications, research focus has been mainly on the investigations of the effects of embedment of nanostructures on the physical properties of the CN sheets [4]. However, the understanding of the mechanical properties and modulation of the electronic properties of these stable (heptazine and s-triazine) sheets remain unclear. In the present work [5,6], we investigate the mechanical properties and electronic properties modulations under symmetric deformations of both heptazine and s-triazine sheet based on density functional theory [7] calculations with the aid of Quantum ESPRESSO package [8]. Our results show that the in-plane stiffness and bulk modulus for s-triazine sheet are less than that of heptazine sheet. The decrease in value can be related to the nature of the covalent bonds linking the adjacent sheets and the number of atoms per unit cell. The Poisson's ratio of s-triazine sheet is in the same order of magnitude to that for heptazine sheet. The calculated values of the two critical strains (elastic and yielding points) of s-triazine sheet are in the same order of magnitude to that for heptazine which was calculated using MD simulations [9]. It is also shown that heptazine and s-triazine sheets can withstand larger tension in the plastic region. These results established a stable mechanical property for s-triazine and heptazine sheets. We also found a linear relationship of bandgap as a function of bi-axial tensile strain within the harmonic elastic region. The reduced steric repulsion of the lone pairs (p_x , p_y) causes the p_z -like orbital to shift to high energy, and consequently an increase in the bandgap. We find no change in electronic properties of the heptazine and s-triazine sheets under electric field up to a maximum value of 10 V/nm. These promising properties may offer opportunities in future material applications.

References

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Figures

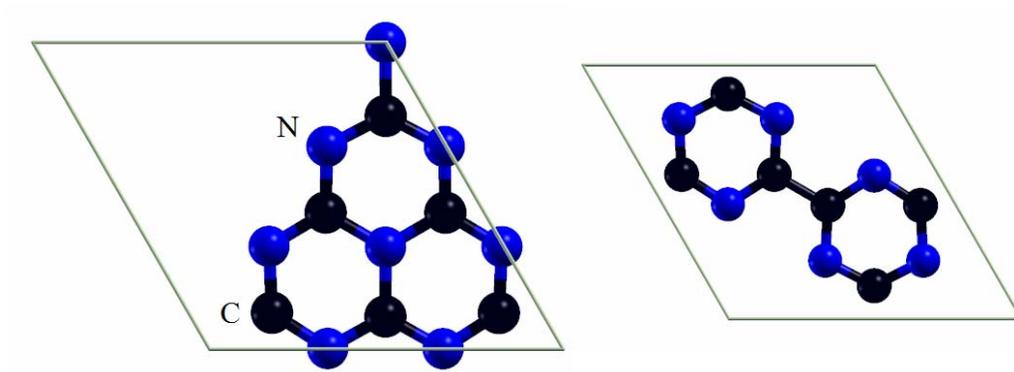


Figure 1: Optimized structure of heptazine (left panel) and s-triazine (right) sheets