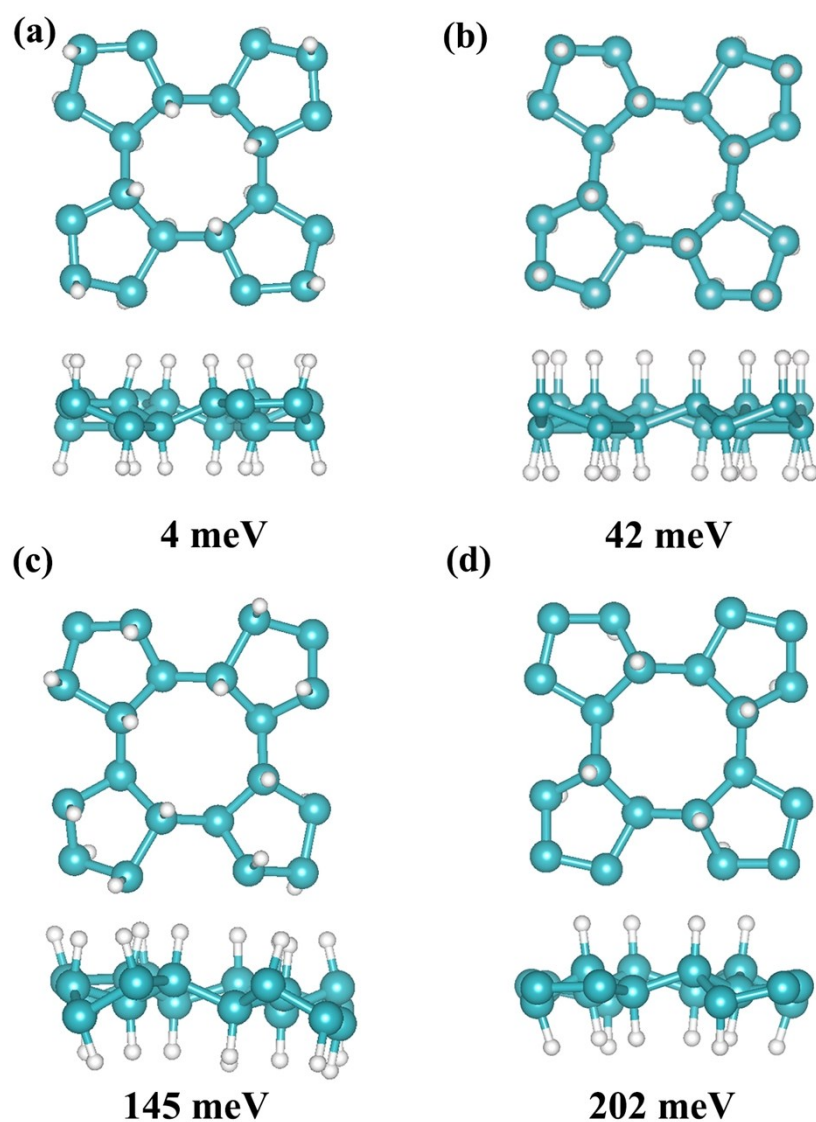
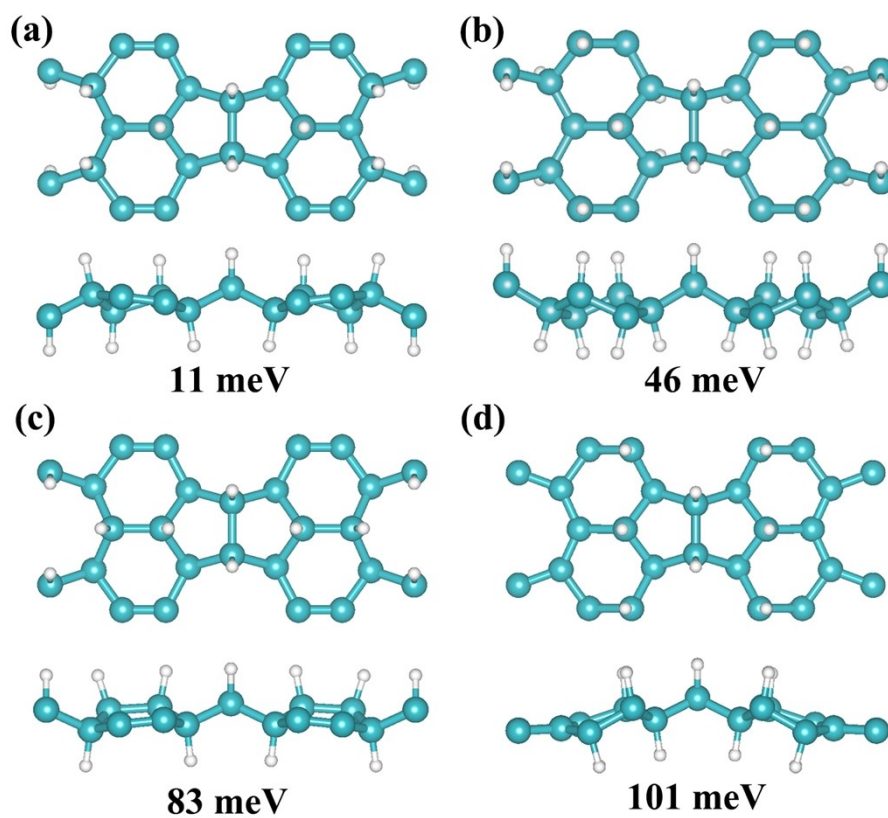


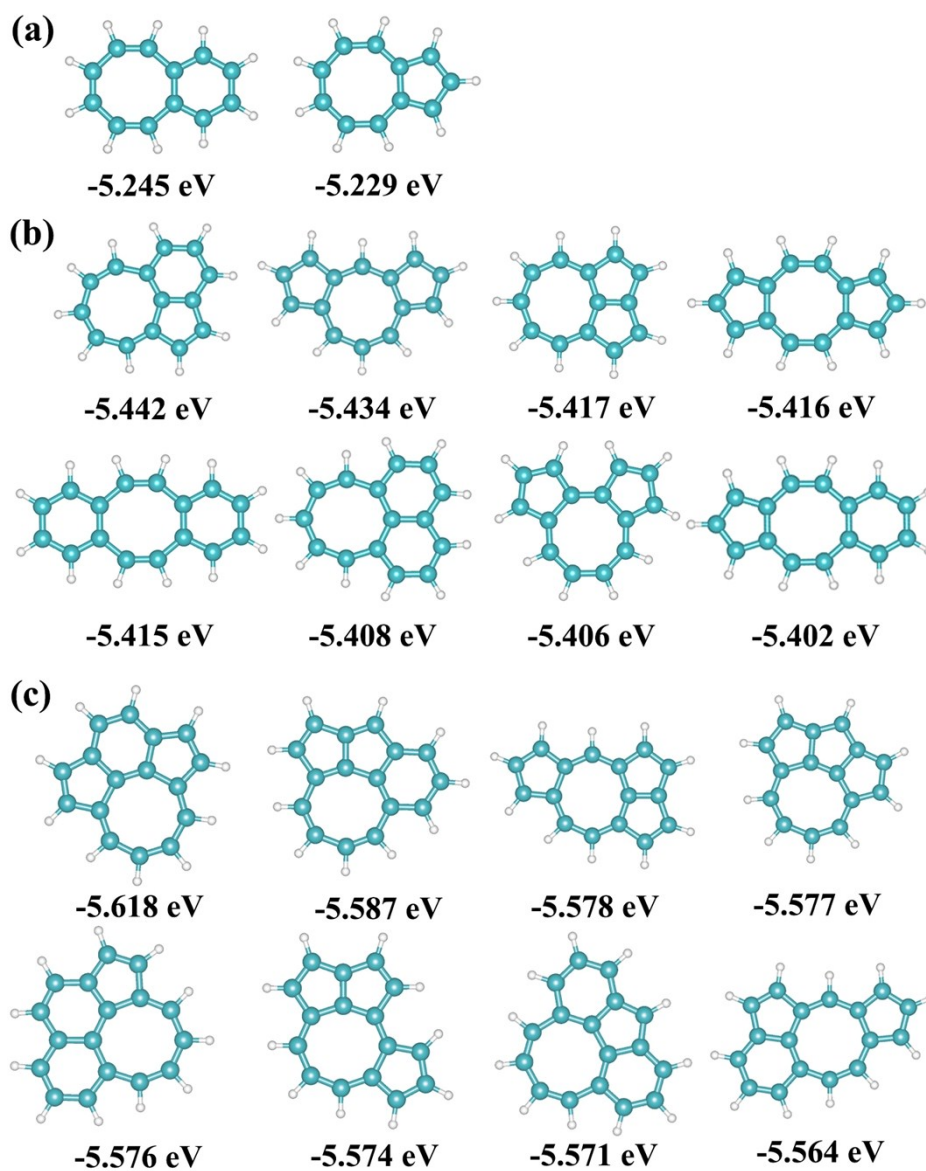
## Supplementary Materials



**Figure S1** The first four low-lying isomers of the hydrogenated  $\alpha$ -phagraphene with the relative energies per H atom as referred to the lowest hydrogenation configuration. The cyan and white balls stand for the carbon and hydrogen atoms, respectively. Both top and side views of each configuration are presented.



**Figure S2** The first four low-energy isomers of the hydrogenated  $\beta$ -phagraphene with the relative energies per H atom as referred to the lowest hydrogenation configuration. The cyan and white balls stand for the carbon and hydrogen atoms, respectively. Both top and side views of each configuration are presented.



**Figure S3** The structural motifs of the phographene with the total energies per atom provided below each structure. The (a), (b), and (c) are the configurations containing 2, 3, and 4 carbon rings, respectively. The cyan and white balls stand for the carbon and hydrogen atoms, respectively.