Supplementary Material

New carbon allotrope in orthorhombic symmetry via graphitic sheet buckling

Figure S1(a) shows the calculated total energy as a function of volume for O_{32} carbon, compared to the results for *M*, *W*, *O*, and *Z*-carbon under GGA method. We can see that O_{32} carbon is energetically more stable than other cold-compressed graphite phases, and the energetic data establish the stability sequence: *M*<*W*<*O*<*Z*<O_{32} carbon. These results are consistent with the LDA data given in Fig. 1(b). The enthalpy-pressure relations under GGA are also presented in Fig. S1(b), and it is shown that O_{32} carbon is more favorable than graphite above 14.25 GPa.

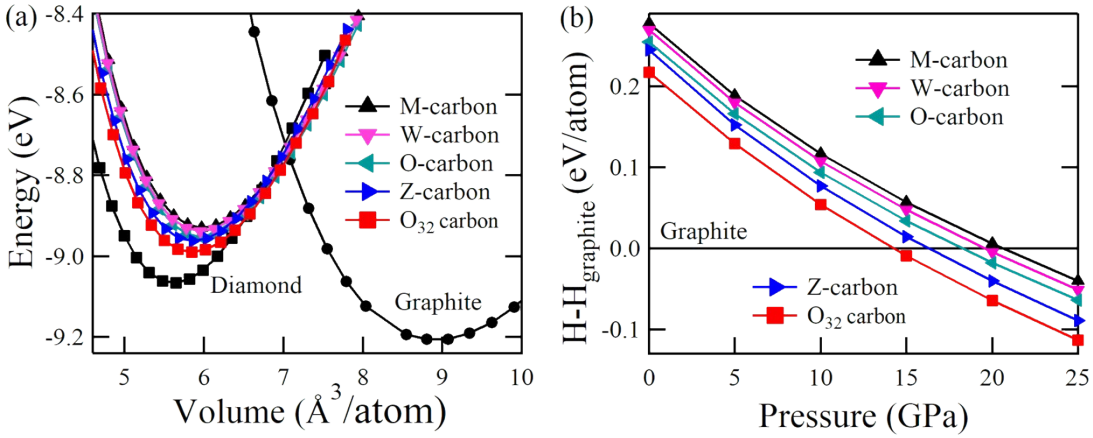

Fig. S1 (a) Total energy as a function of volume for graphite, diamond, *M*-carbon, *W*-carbon, *O*-carbon, *Z*-carbon, and O_{32} carbon. (b) The enthalpy-pressure relations for O_{32} carbon and other cold-compressed graphite phases with respect to graphite. The GGA method is adopted in Fig. S1(a) and Fig. S1(b).