Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

TE-C36 carbon: a new semiconducting phase with an all-sp^3 bonding network

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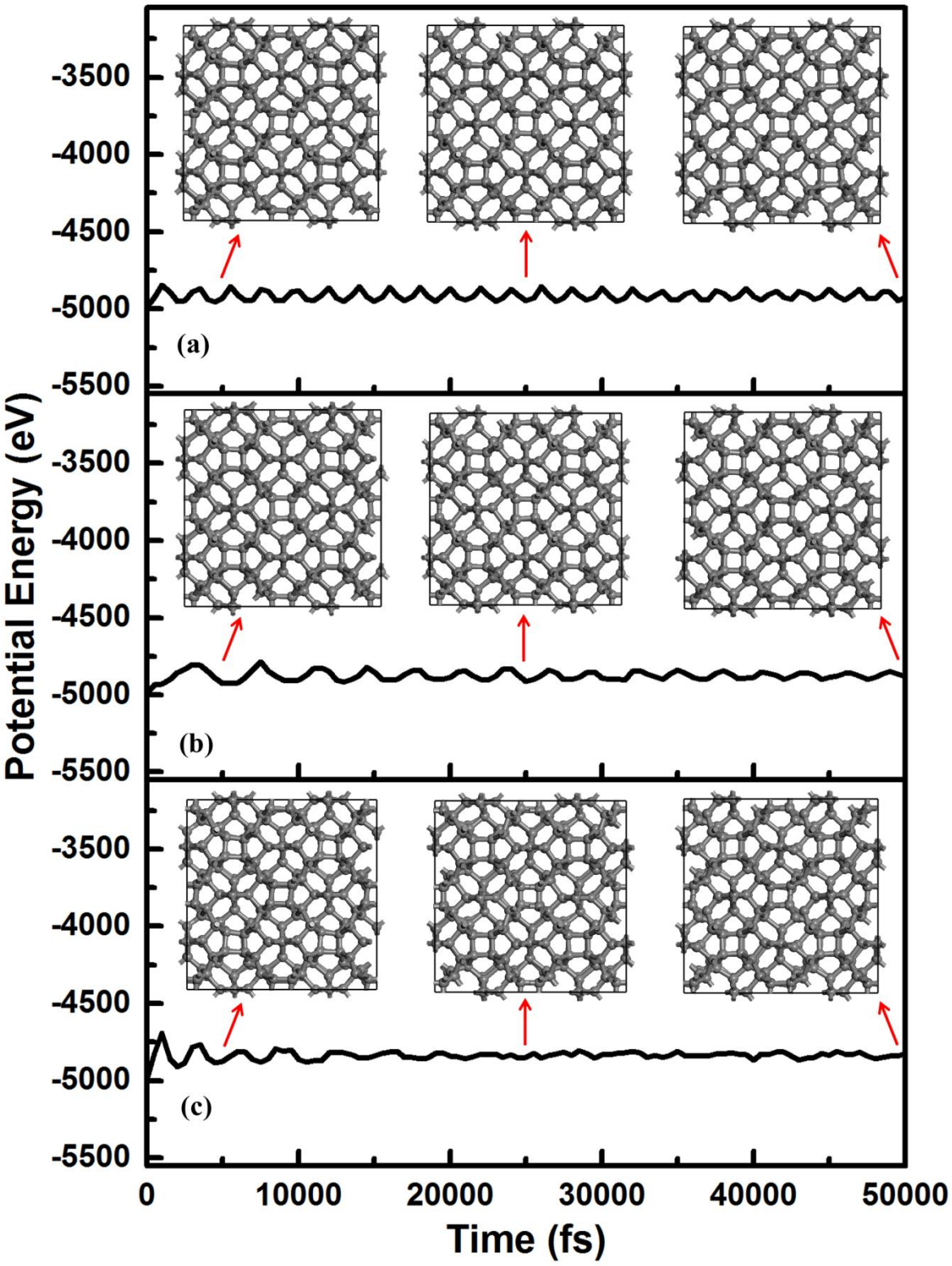

Fig. S1 Potential energy fluctuations of TE carbon in MD simulation at (a) 1000 K, (b) 1500 K and (c) 2000 K. The insets are the snapshots during the MD process.

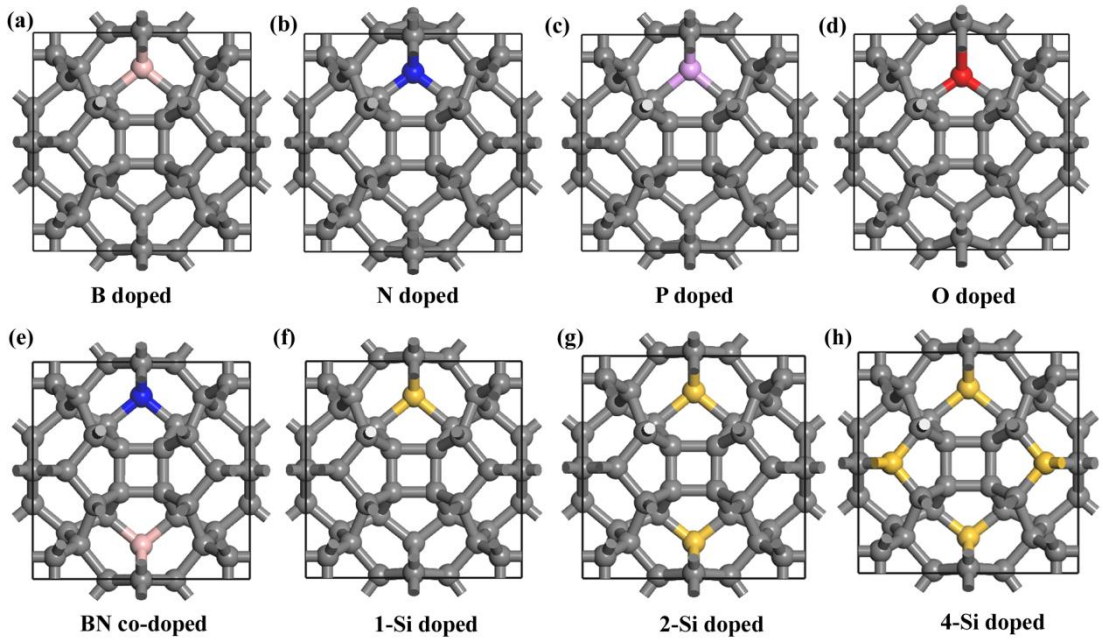

Fig. S2 (a) B doped TE carbon. (b) N doped TE carbon. (c) P doped TE carbon. (d) O doped TE carbon. (e) BN co-doped TE carbon. (f) One Si atom doped TE carbon. (g) Two Si atoms doped TE carbon. (h) Four Si atoms doped TE carbon.

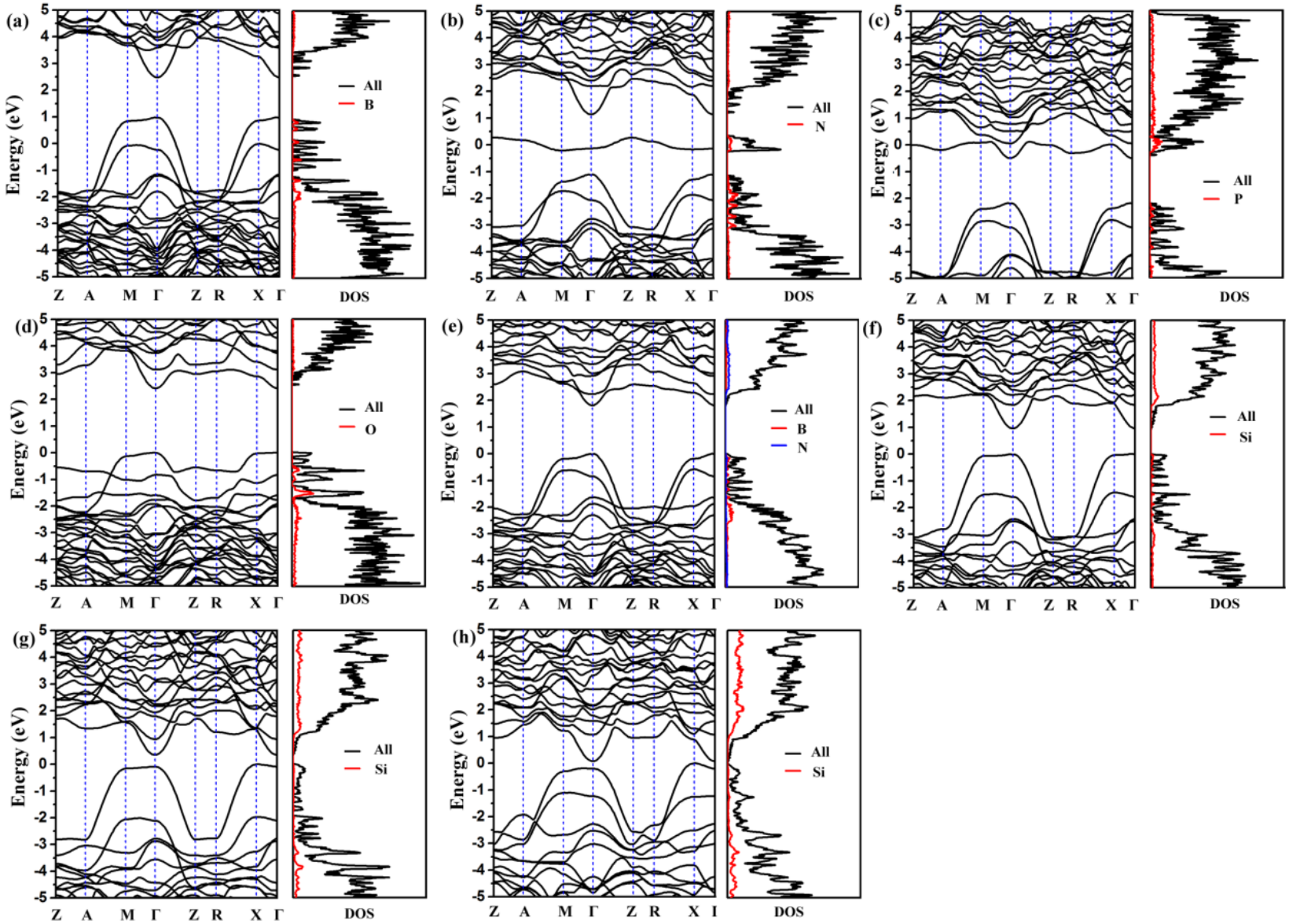

Fig. S3 (a)-(h) Band structures and partial density of states (DOS) for the doped structures in Fig. S2, respectively. Fermi level is set to zero. Z(0,0,0), A(0.5,0.5,0.5), M(0.5,0.5,0), Γ(0, 0, 0), R(0,0.5,0.5), X(0,0.5,0).