Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Doping penta-graphene and hydrogenation of its related structures: a structural and electronic DFT-D study

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Table S1. Relaxed unit cells of all studied structures, and fractional coordinates of parent penta-C structure.

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Table S1. Relaxed unit cells of all studied structures.

Compound	a =b (Å)	c (Å)
penta-C	3.6386	15.0147
H-penta-C	3.4897	17.5589
penta-C-Si	4.4105	16.6516
H-penta-C-Si	4.2179	18.2827
penta-C-Ge	4.5986	16.762
H-penta-C-Ge	4.4088	18.5143
penta-C-Sn	4.8856	16.285
H-penta-C-Sn	4.689	18.783

In red colour is indicated instable structures.

Fractional coordinates of parent penta-C. In table S1 are given its cell parameters.

C 0.000 0.000 0.449
C 0.629 0.869 0.490
C 0.500 0.500 0.449
C 0.369 0.129 0.490
C 0.869 0.369 0.409
C 0.129 0.629 0.409

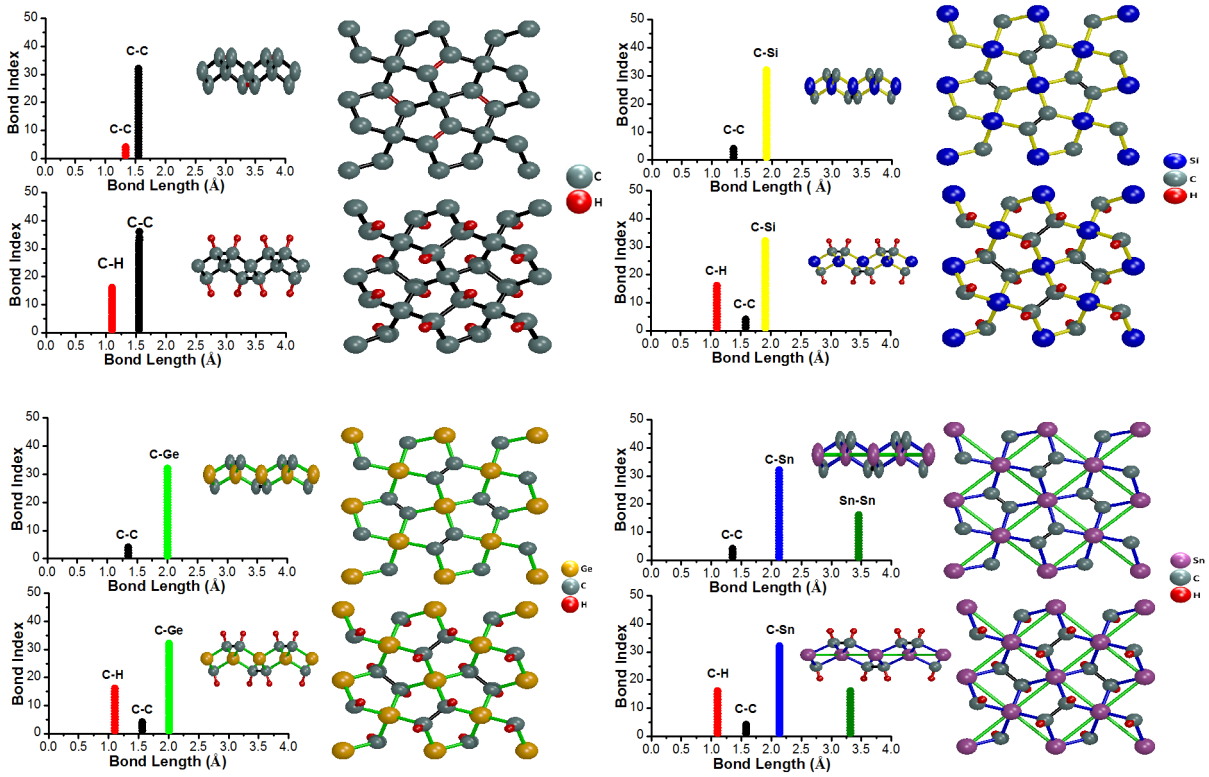

Figure S1. Bond lengths of all studied structures. After hydrogenation C-C bonds suffer of enlargement getting close to the value found in diamond (sp^3 hybridization). Interestingly, in H-penta-C-Sn, Sn-Sn bonds are shorter than in penta-C-Sn structure.

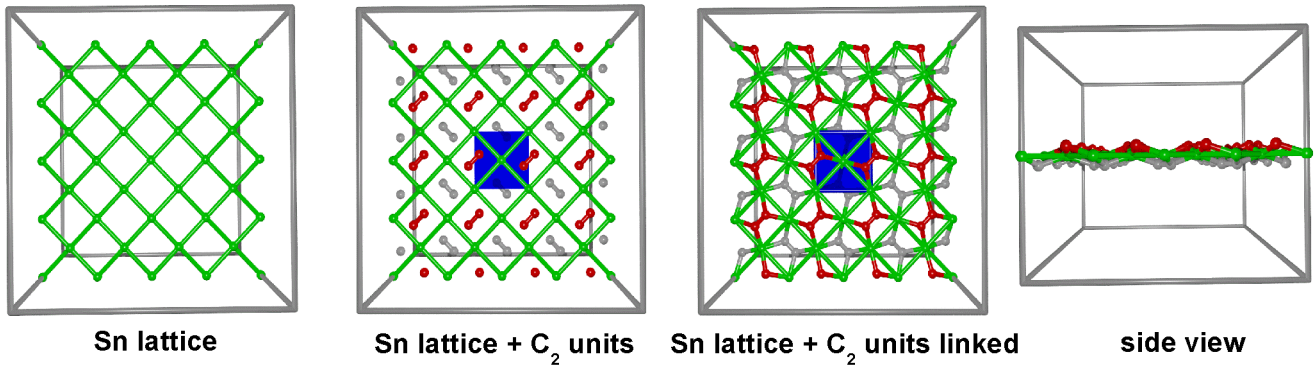

Figure S2. Structure of penta-C doped with Sn atoms. Sn, and C atoms are displayed in green and gray/red colors. Side view clearly shows that C atoms are distributed on both sides of the Sn lattice forming C_2 units. In blue color is shown the translational cell.

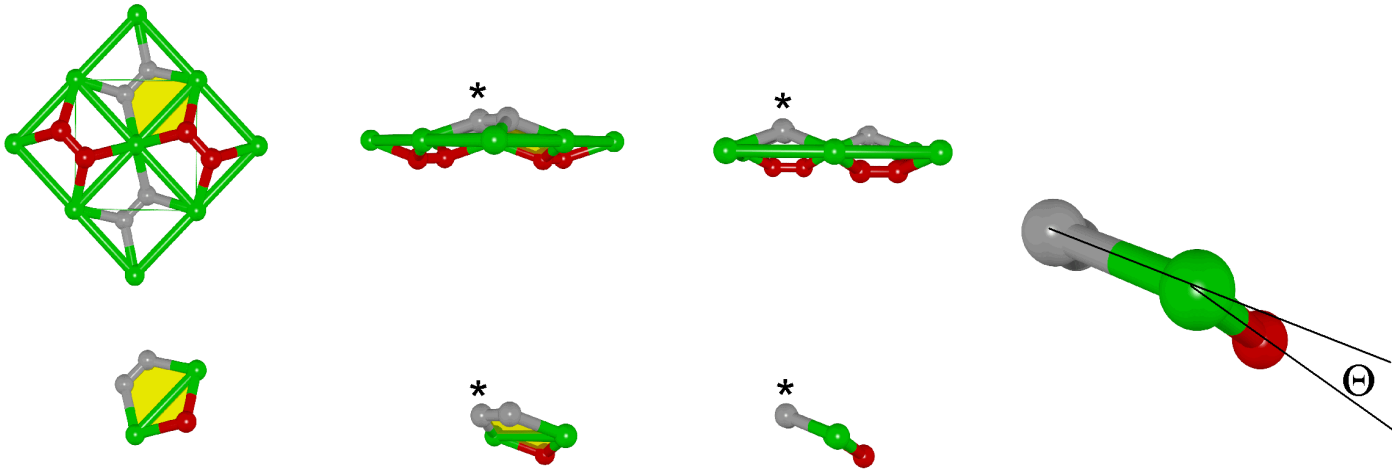

Figure S3. Procedure to choose an irregular pentagonal ring of penta-C-Sn structure. Asterisks are used as a visual help on two orientations of the same 2D layer. Middle frame on the right side shows the deflection angle (θ) of an irregular pentagonal ring. Noteworthy is that all the irregular pentagonal rings are equal and related by symmetry along the 2D framework.

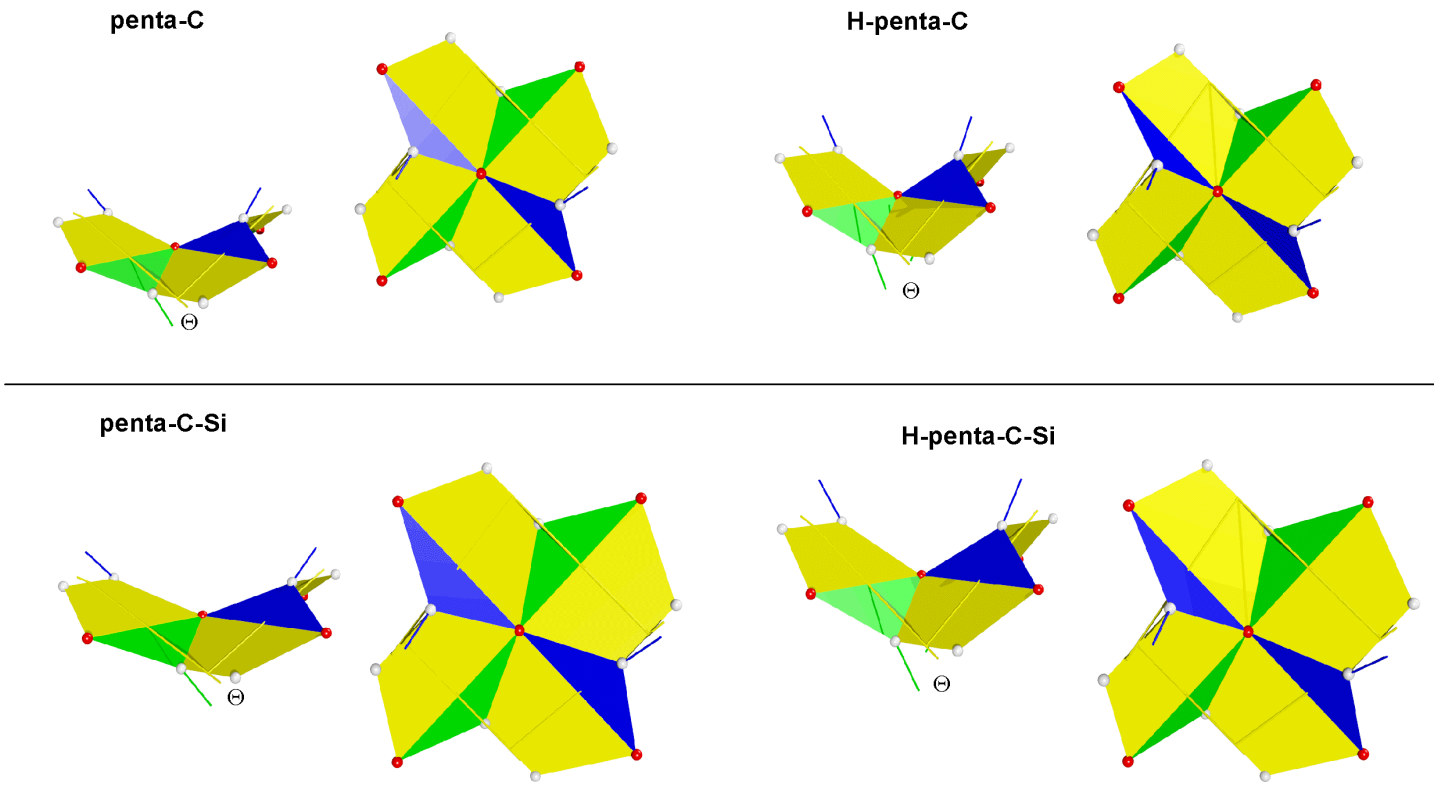

Figure S4. Major deflection angles found among all the studied structures. Left column corresponds with doped penta-C structures and right column presents hydrogenation of doped structure (penta-graphane). It is evident that after hydrogenation, the deflection angle increases.

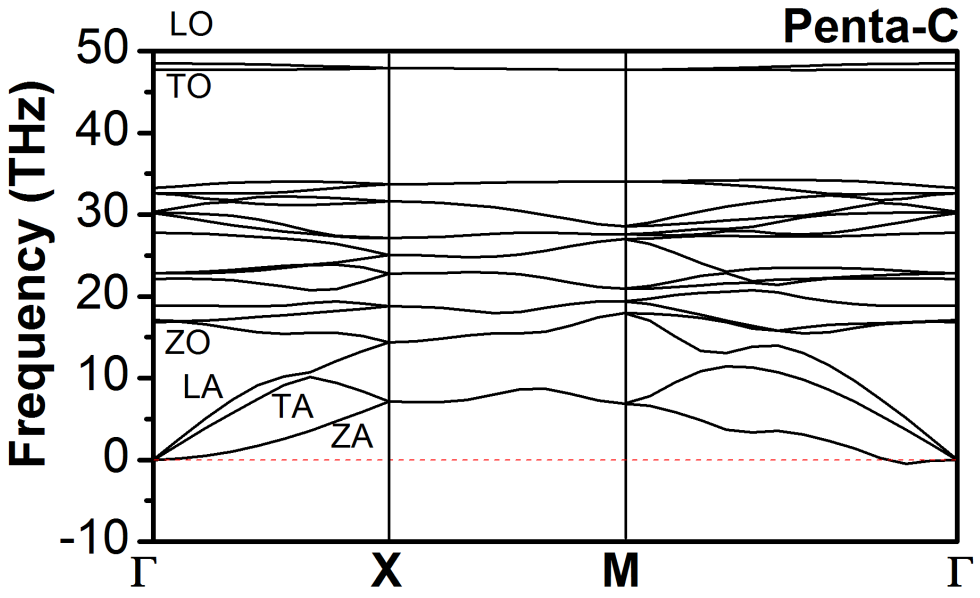

Figure S5. Phonon dispersion of penta-graphene based on GGA-PBE. ZA stands for out-of-plane acoustic banches; TA is transverse acoustic branch; LA is Longitudinal acoustic branch; ZO stands for out-of-plane optizal phonos; TO is transverse optical phonons, and LO is the longitudinal optical branch.

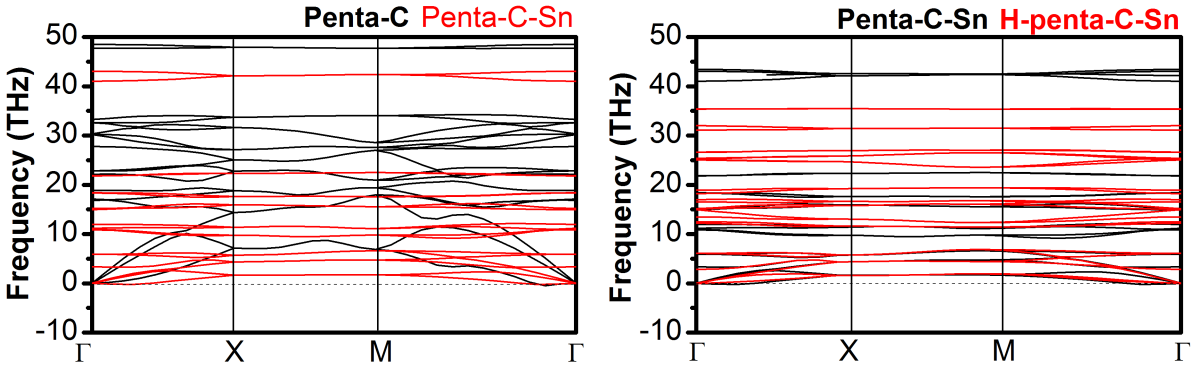

Figure S6. Comparison of Phonon dispersion plots of penta-C against Sn doped penta-C (left panel) and among Sn-doped penta-C and its hydrogenated structure (right panel).

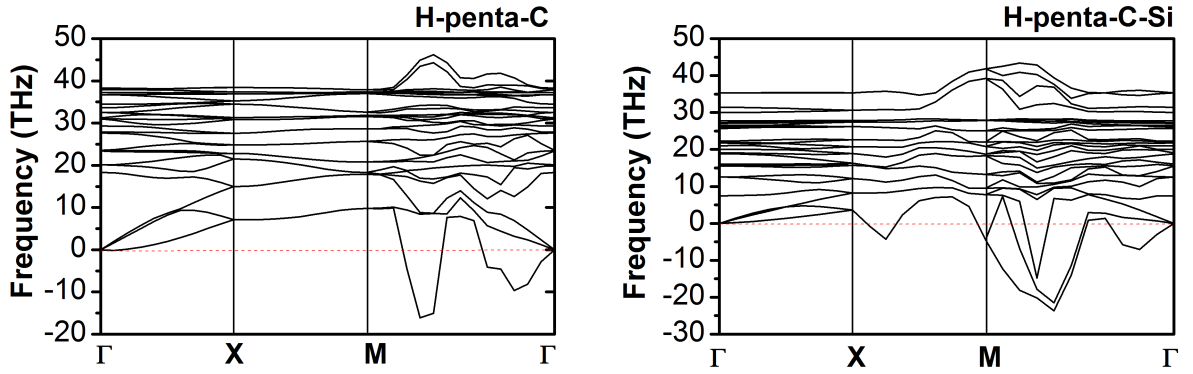

Figure S7. Phonon dispersion plots of instable structures. It is found intense imaginary frequencies along Γ-M direction of hydrogenated structures of penta-C and penta-C-Si.

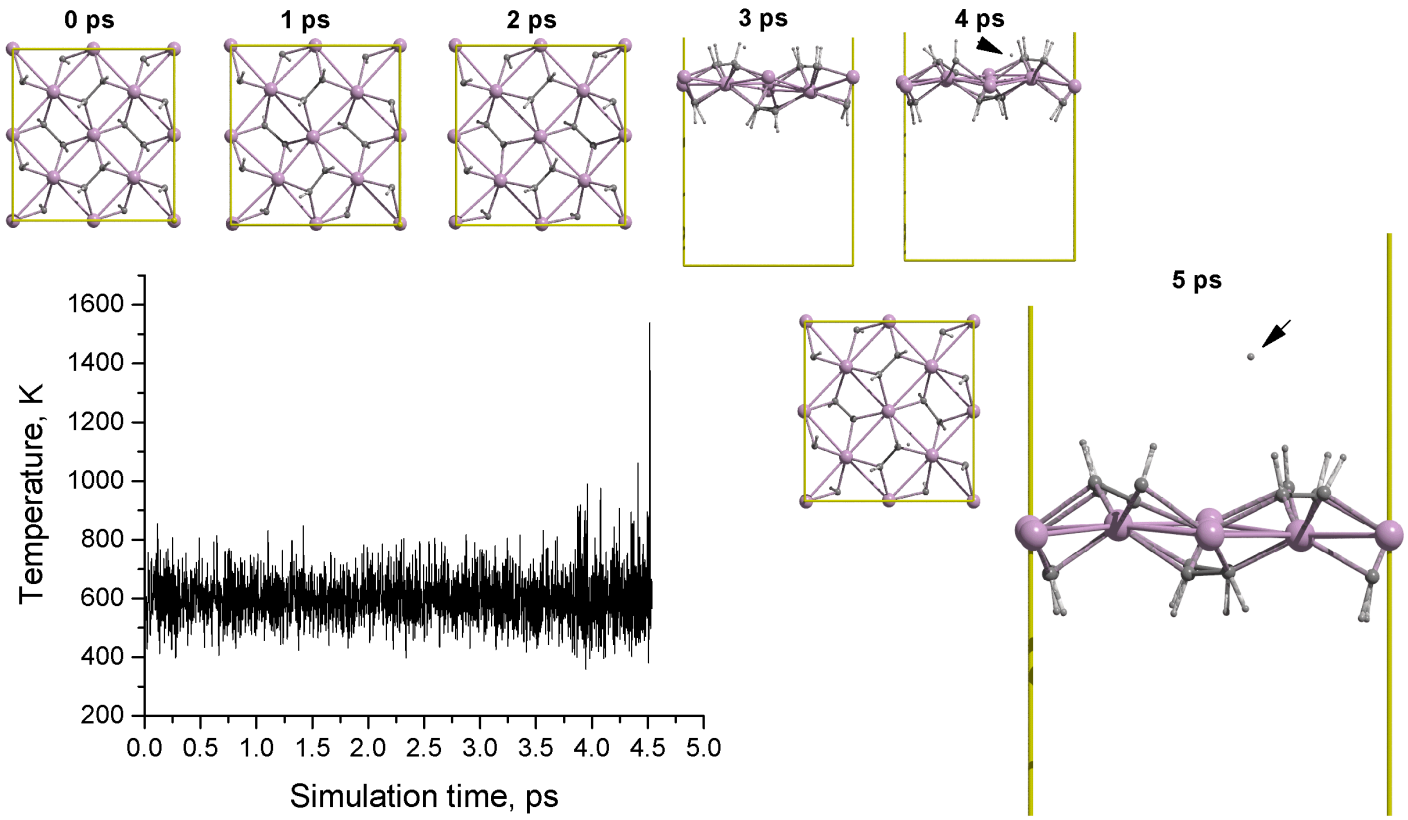

Figure S8. BOMD snapshots for H-Sn-penta-C simulation which was carried out at 600 K and 1 atm. Leaving H atom is indicated with an arrow.

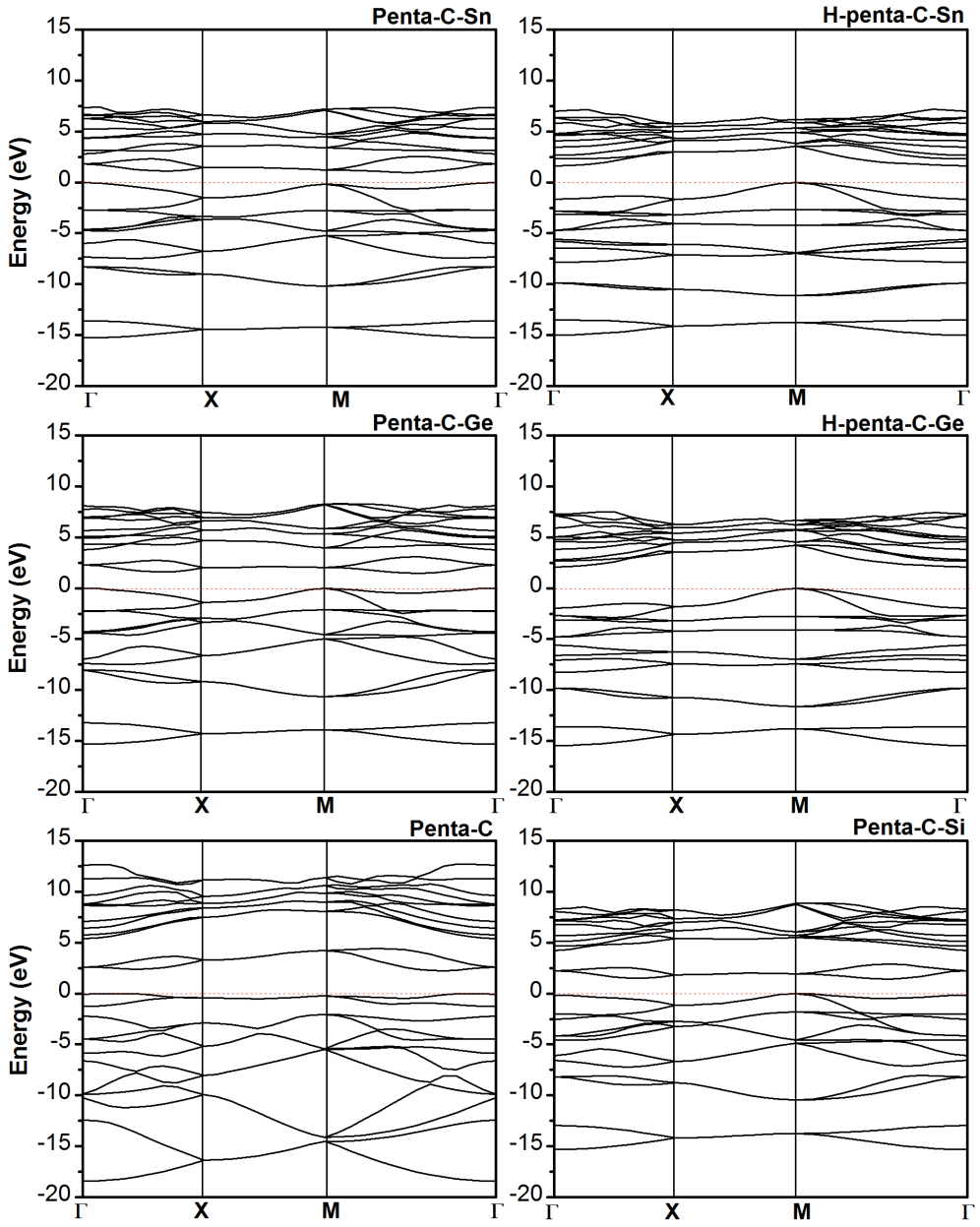

Figure S9. Bands structures of calculated compounds based on PBE functional. Fermi energy is located at zero.

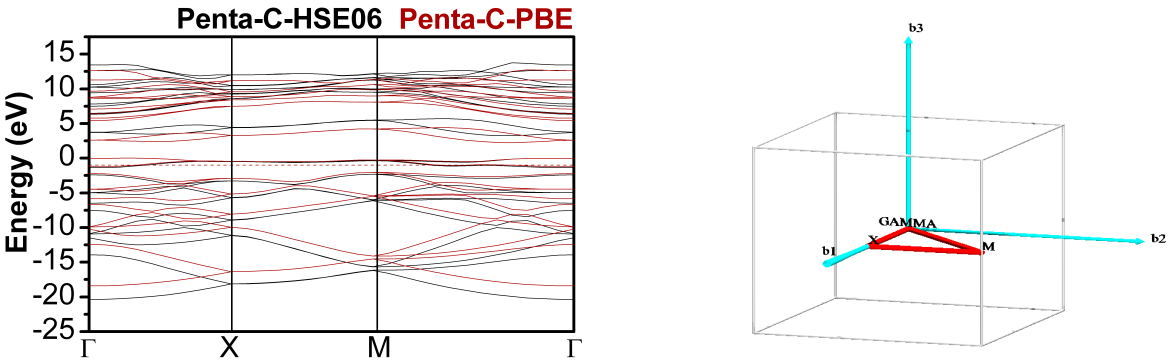

Figure S10. Comparison of bands structure of penta-C based on PBE and HSE06 functionals. Righ panel shows special k points and the directions along them.