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

Supporting Information For

Electronic Structures of Group-V − Group-IV Hetero-bilayer Structures: A First-principles Study

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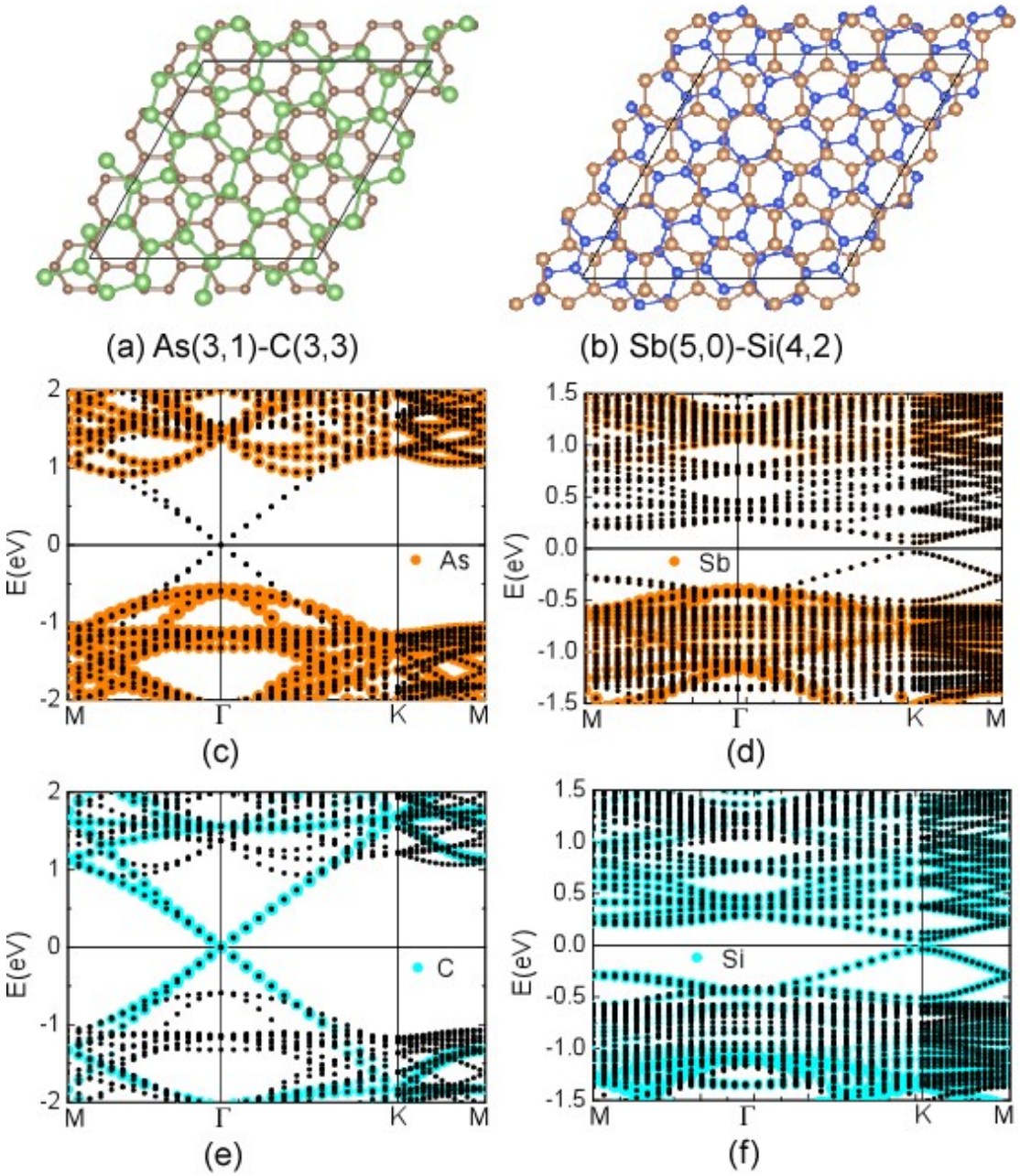

Figure S1: The atomic structures and band structures of [(a),(c),(e)] As(3,1)-C(3,3) and [(b),(d),(f)] Sb(5,0)-Si(4,2) hetero-sheets. The bands projected to As (Sb) and C (Si) orbitals are highlighted by orange and cyan circles, and the size corresponds to the weight of each species in the bands.

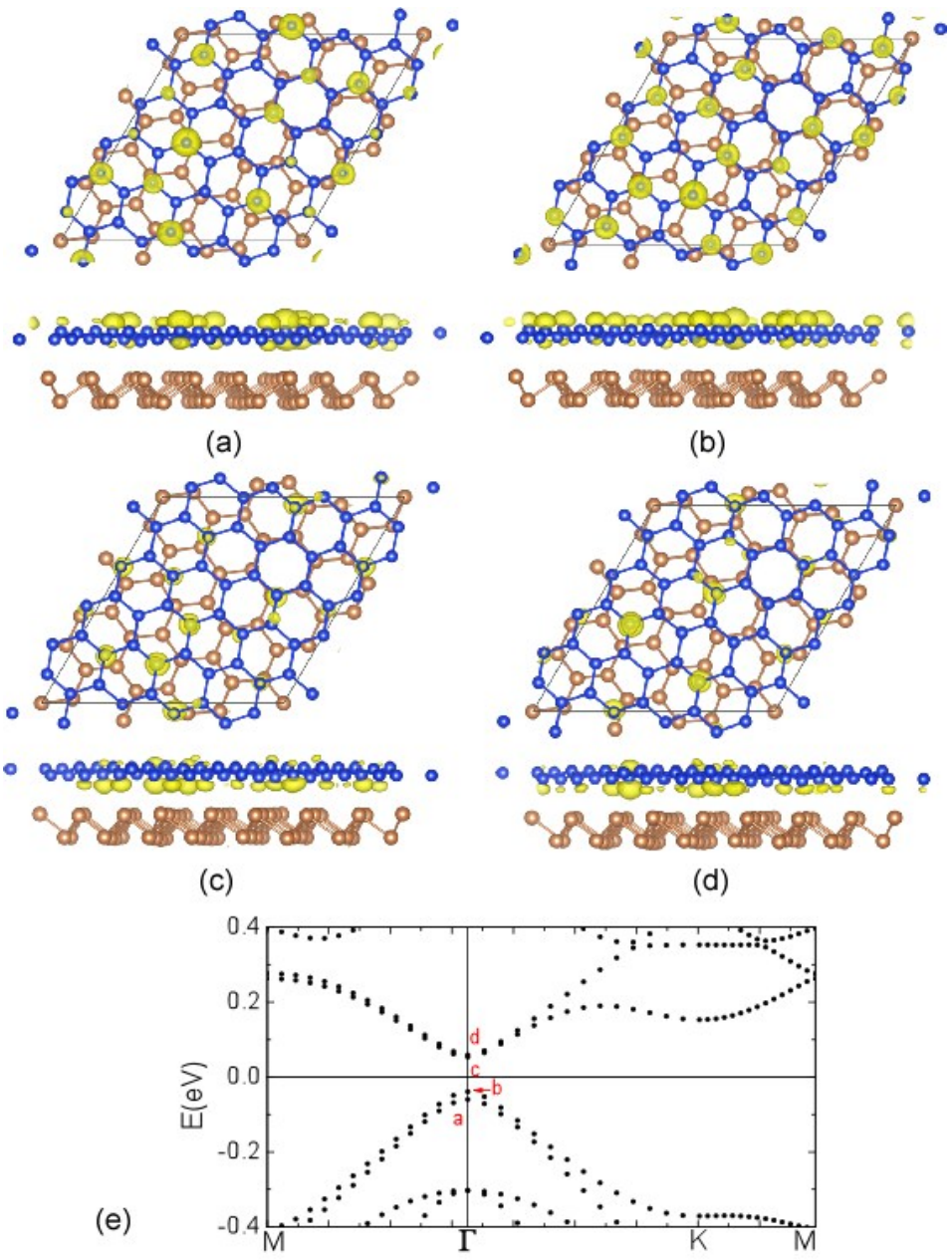

Figure S2: The partial charge densities of [(a),(b)] the valence band states and [(c),(d)] the conduction band states in the Sb-Si hetero-sheet, for which the corresponding energy points are marked in (e).

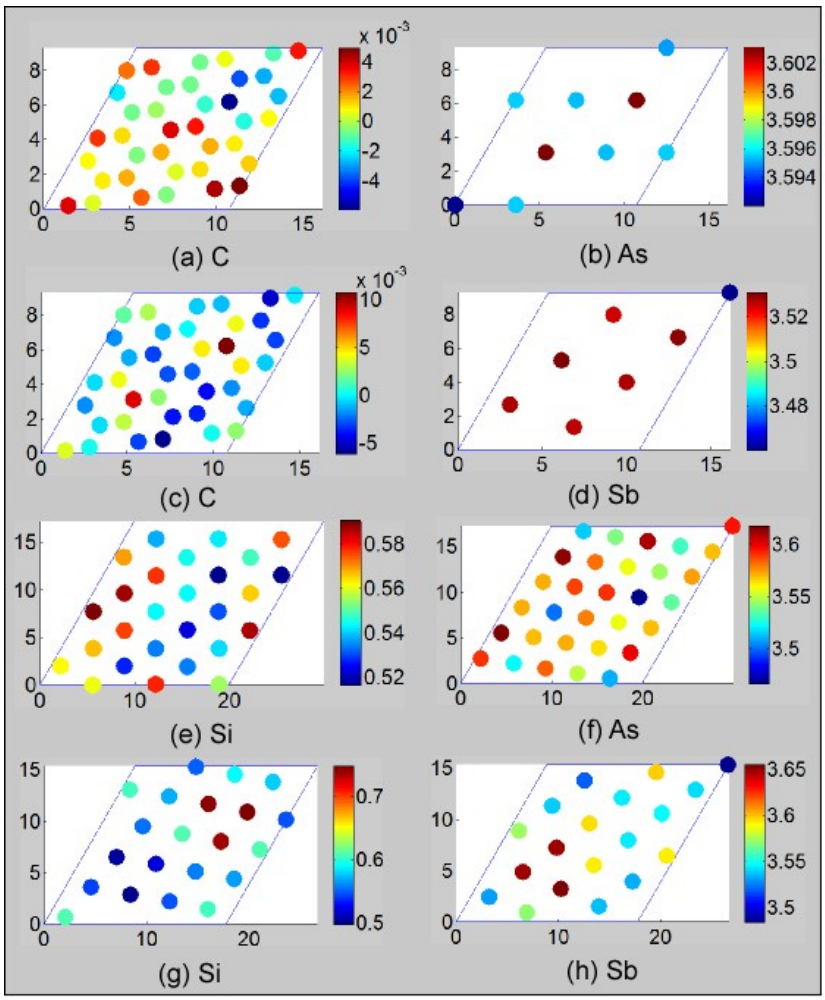

Figure S3: The height distributions of atoms at the inteface of [(a),(b)] As-C,[(c),(d)] Sb-C, [(e),(f)] As-Si, and [(g),(h)] Sb-Si hetero-sheets. Since the As, Sb and Si layers are buckled with a chair-like conformation, only the atoms located at the inside of the hetero-sheets are displayed in the figures.

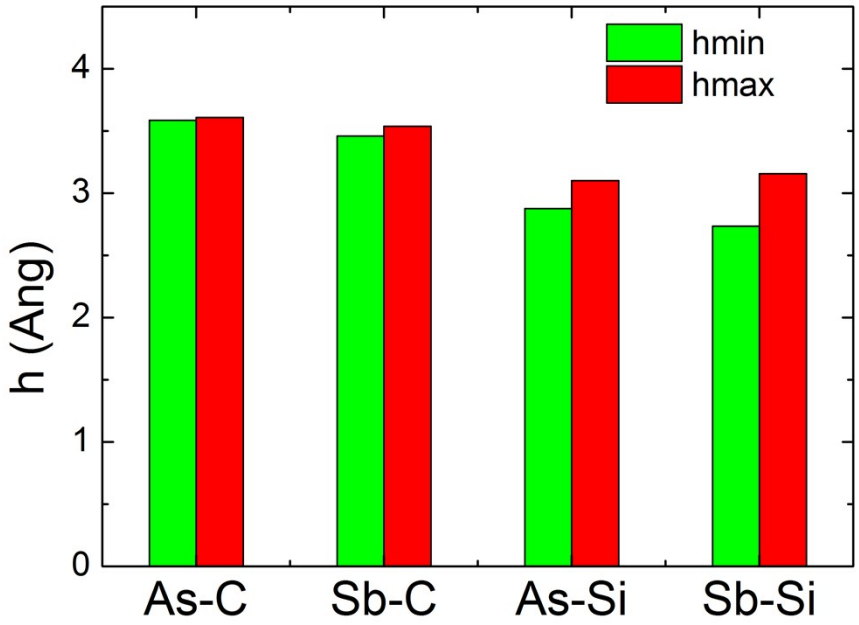

Figure S4. The minimum and maximum values of interlayer distances in the As/Sb-C/Si hetero-sheets.The h_{min} (h_{max}) values are calculated as the differences between the smallest (largerst) height in the upper layer and the largest (smallest) height in the bottom layer. Since the interlayer distance is determined by the atoms at the interface region of hetero-sheets, only the atoms at the interface are considered for the buckled As,Sb, Si layers.

	Top	Hollow	Bridge
As-C heterosheet	1.02	***0***	0.69
Sb-C heterosheet	6.22	***0***	3.98
As-Si heterosheet	11.49	0	***-2.67***
Sb-Si heterosheet	25.33	***0***	5.19

Table. S1: The relative energies for the top, hollow, and bridge site conformations of As/Sb-C/Si hetero-sheets. Here, the energy of hollow site conformation is used as a reference in each hetero-sheet. The unit is meV per supercell in the table. The smallest value, which is marked in a bold Italic, corresponds to the most stable conformation of the hetero-sheet.