Supporting Information

Exploration of Structures of Two-Dimensional Boron-Silicon Compounds with sp^2 Silicon

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TABLE S1 Calculated cohesive energies for the predicted low-energy monolayer structures of B-Si compounds. The unit is meV/atom.

	I	II	III
BSi_4	4232.7	4137.7	4129.5
BSi_3	4307.0		
BSi_2	4443.0	4421.9	
BSi	4671.2	4666.1	
B_2Si	5263.3	5203.5	5188.2
B_3Si	5355.5		
B_4Si	5502.3	5485.5	5478.3
B_5Si	5547.6	5547.3	
B_6Si	5600.1	5566.1	5560.7
B_7Si	5686.3	5664.2	

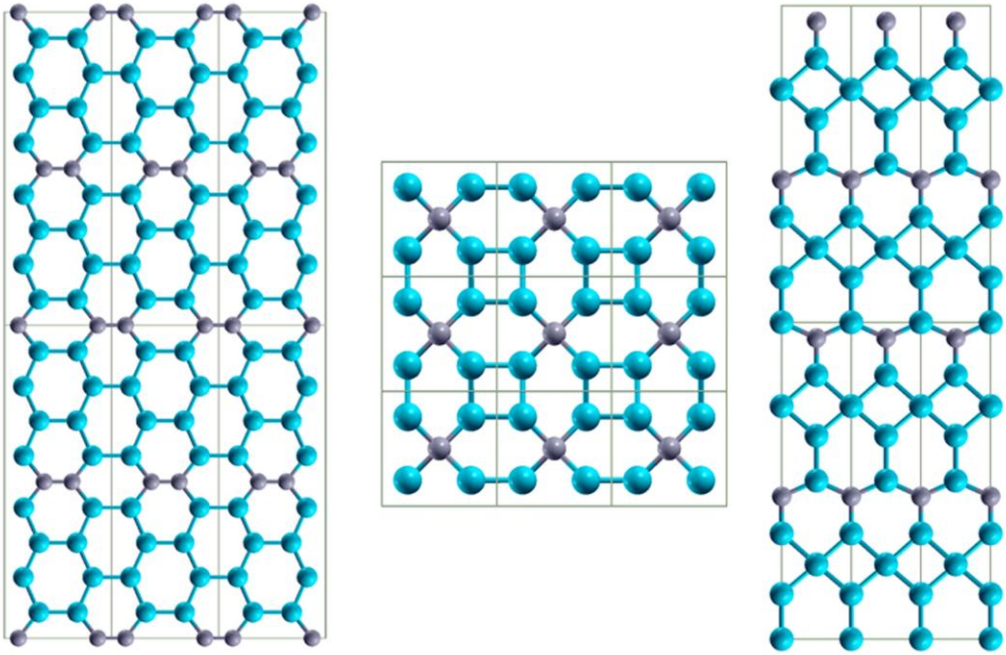

Figure S1: Low-energy monolayer structures of BSi_4 from the PSO search.

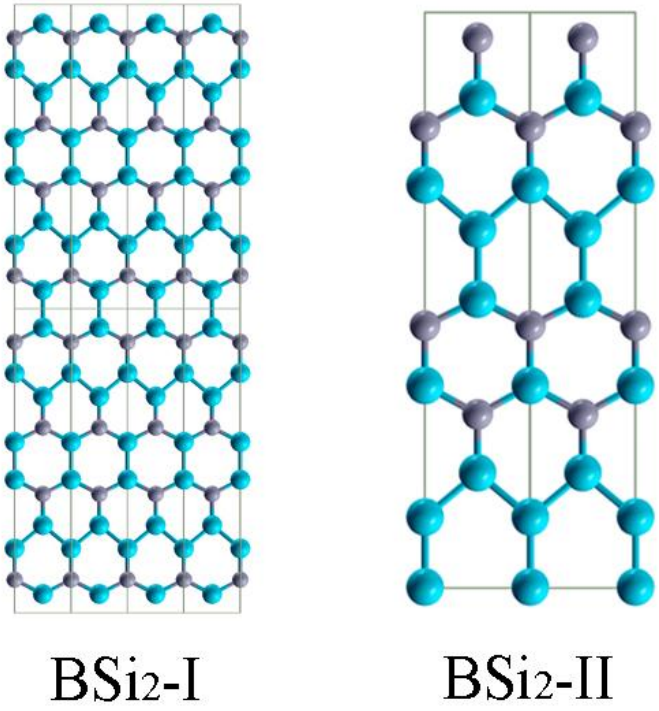

Figure S2: Low-energy monolayer structures of BSi_2 from PSO search.

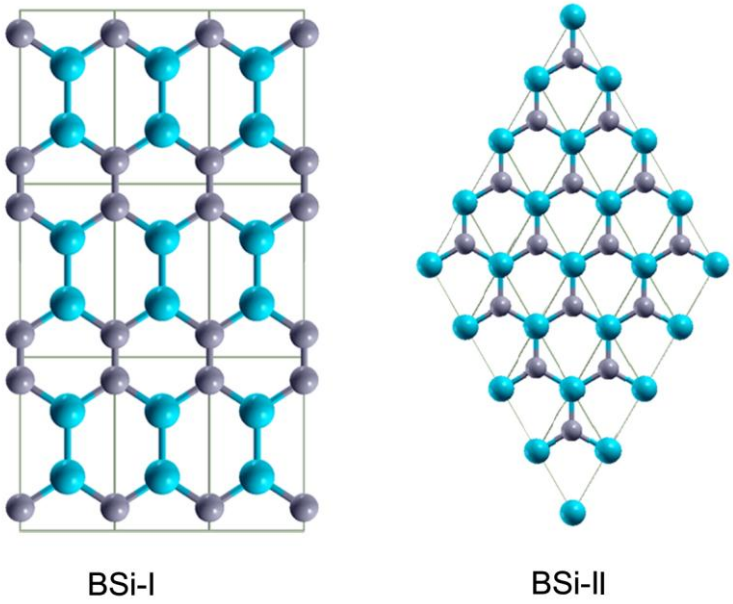

Figure S3: Low-energy monolayer structures of BSi from PSO search.

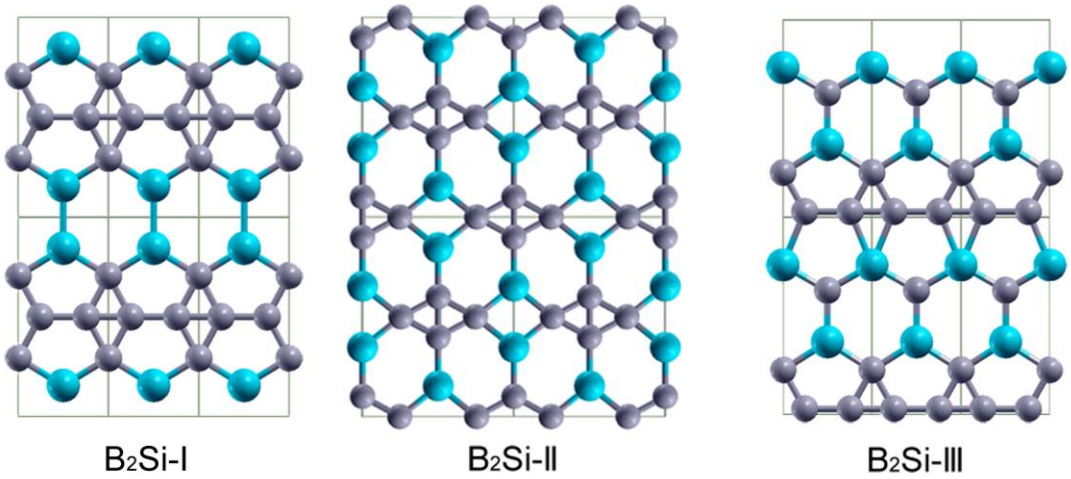

Figure S4: Low-energy monolayer structures of B_2Si from PSO search.

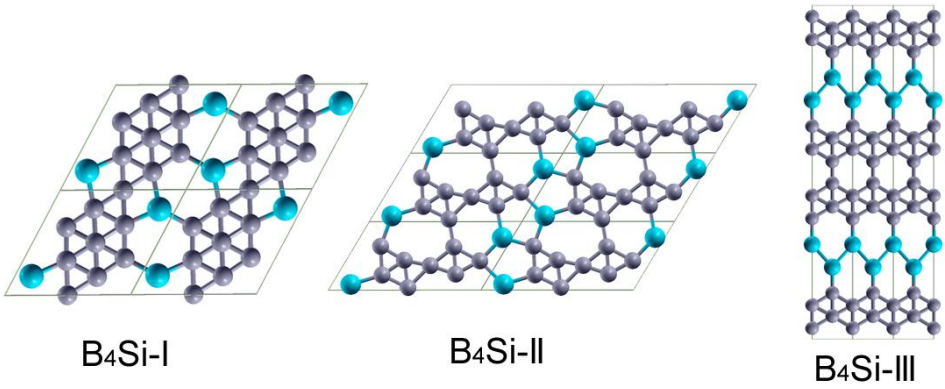

Figure S5: Low-energy monolayer structures of B_4Si from PSO search.

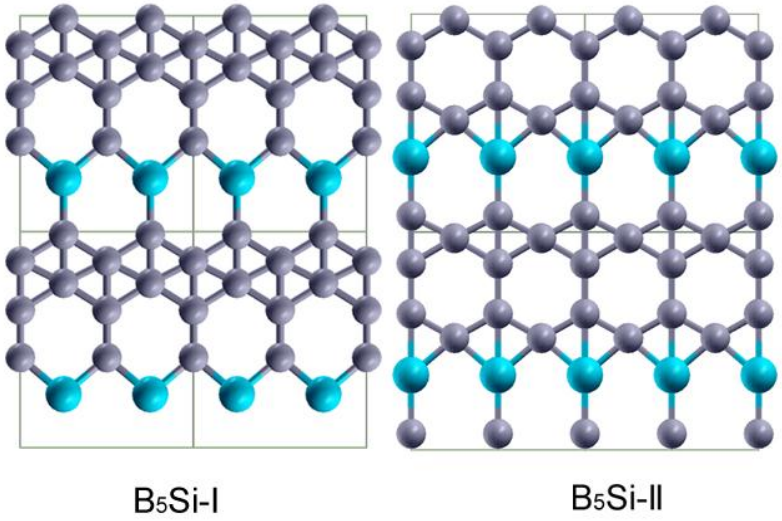

Figure S6: Low-energy monolayer structures of B_5Si from PSO search.

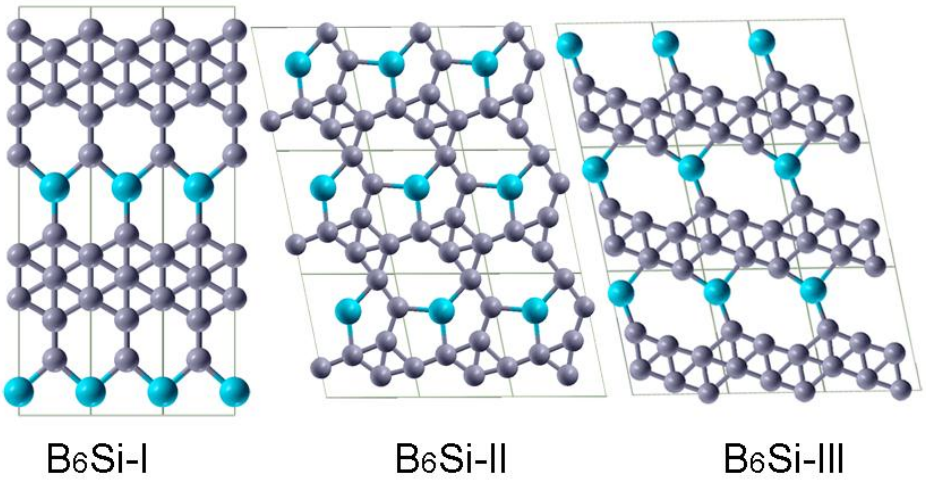

Figure S7: Low-energy monolayer structures of B_6Si from PSO search.

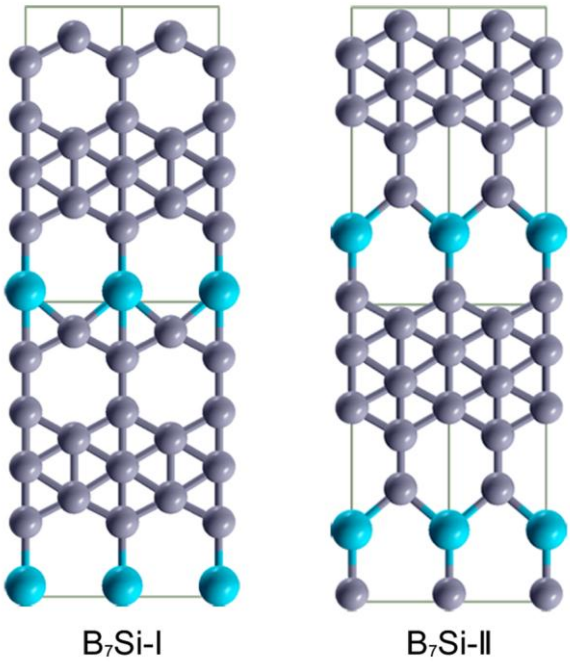

Figure S8: Low-energy monolayer structures of B_7Si from PSO search.

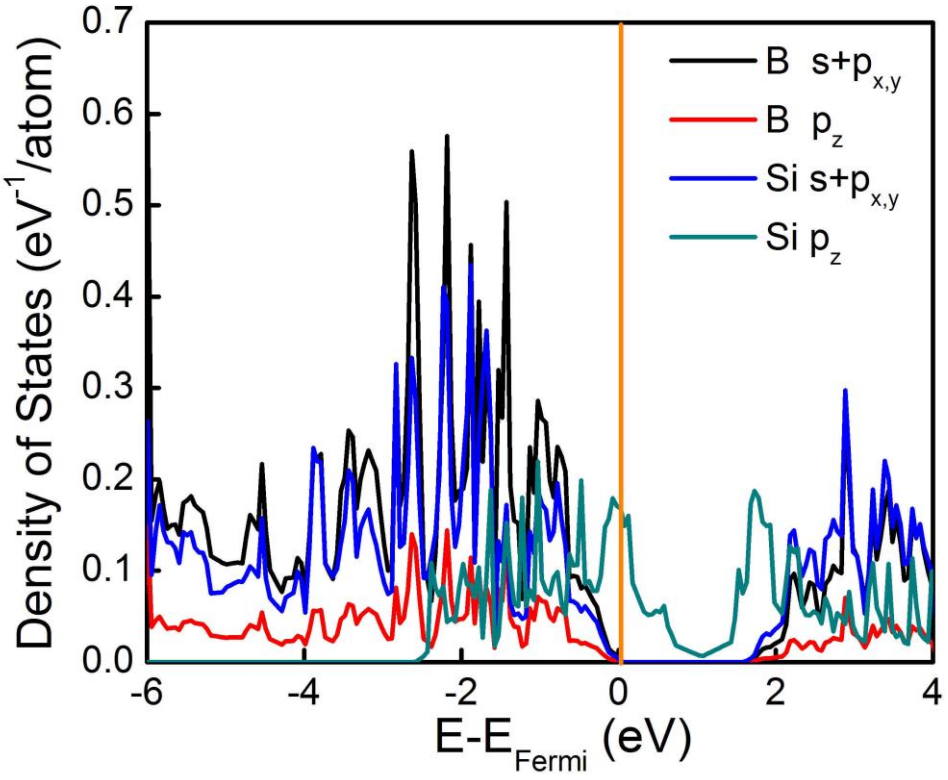

Figure S9: Partial density of states of 2D BSi_4-I.

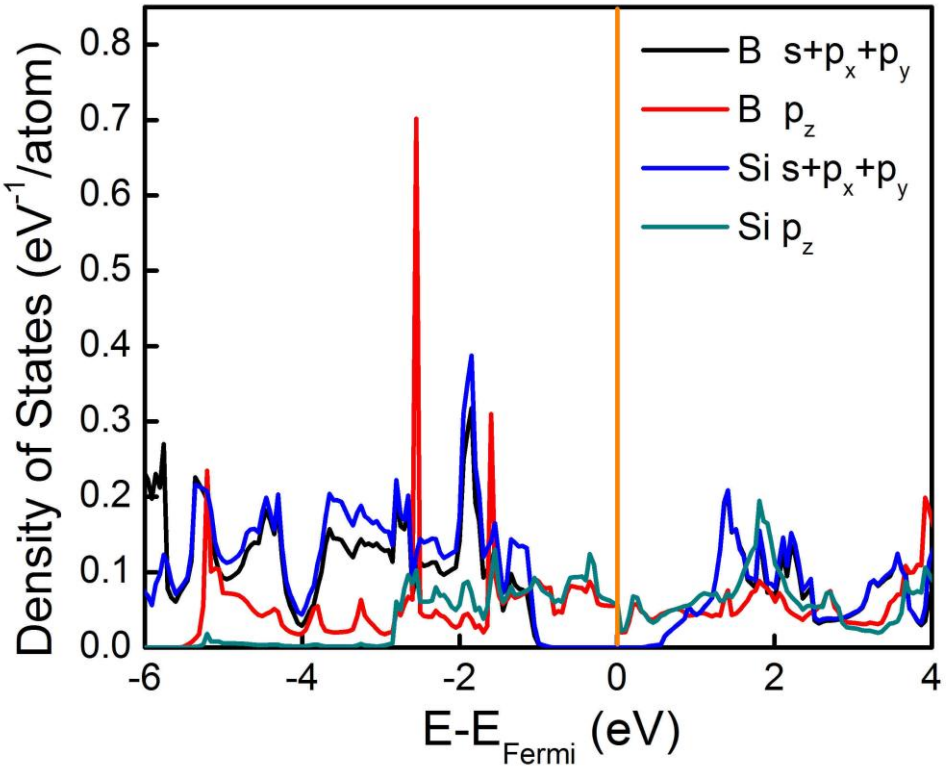

Figure S10: Partial density of states of 2D B_3Si-I.

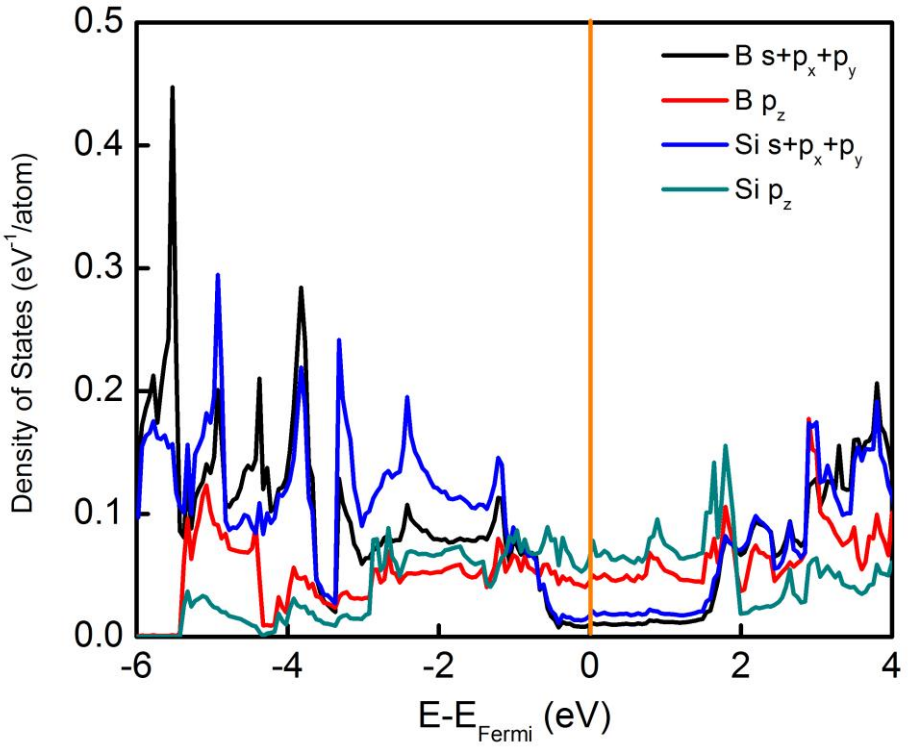

Figure S11: Partial density of states of 2D B_4Si-I.

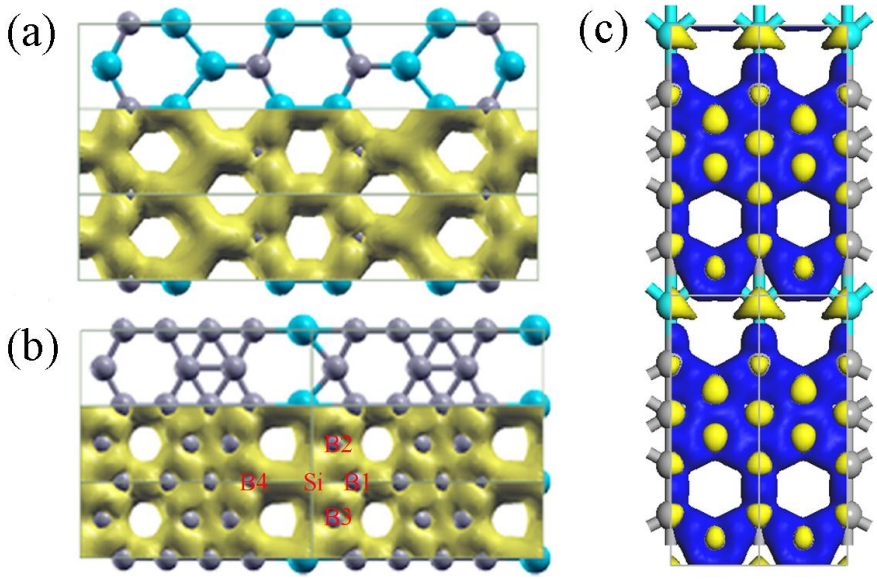

Figure S12: Computed iso-surfaces of electron localization function (ELC) with the value of 0.5 for (a) BSi_2-I and (b) B_7Si-I. (c) Iso-surface (0.05 e/au) of the computed deformation electron density for B_7Si-I, where blue and yellow region refers to electron rich and deficient, respectively.