Supplementary materials for "Computational discovery of two-dimensional tetragonal group IV-V monolayers"

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Content

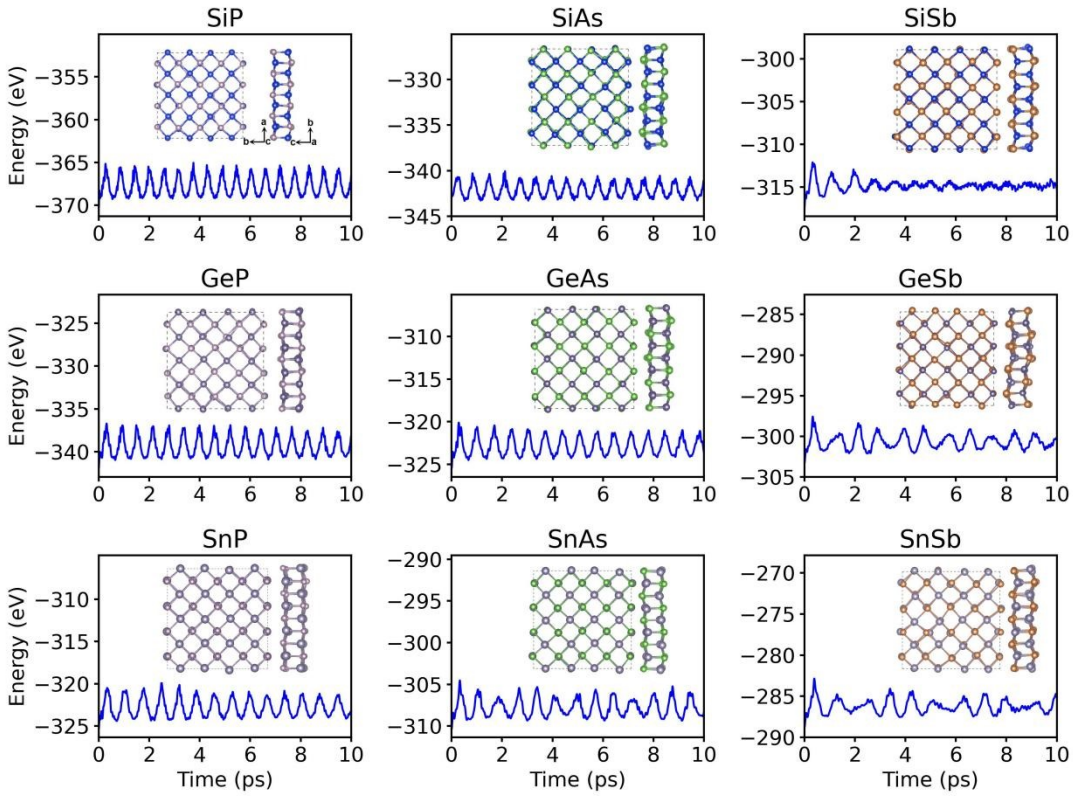

Fig.S1 The fluctuations of the total energy of Td4-phase group IV-V monolayers during the AIMD simulations at 300K; the insets show the final structures of the 2D group IV-V monolayers at the end of the simulation.

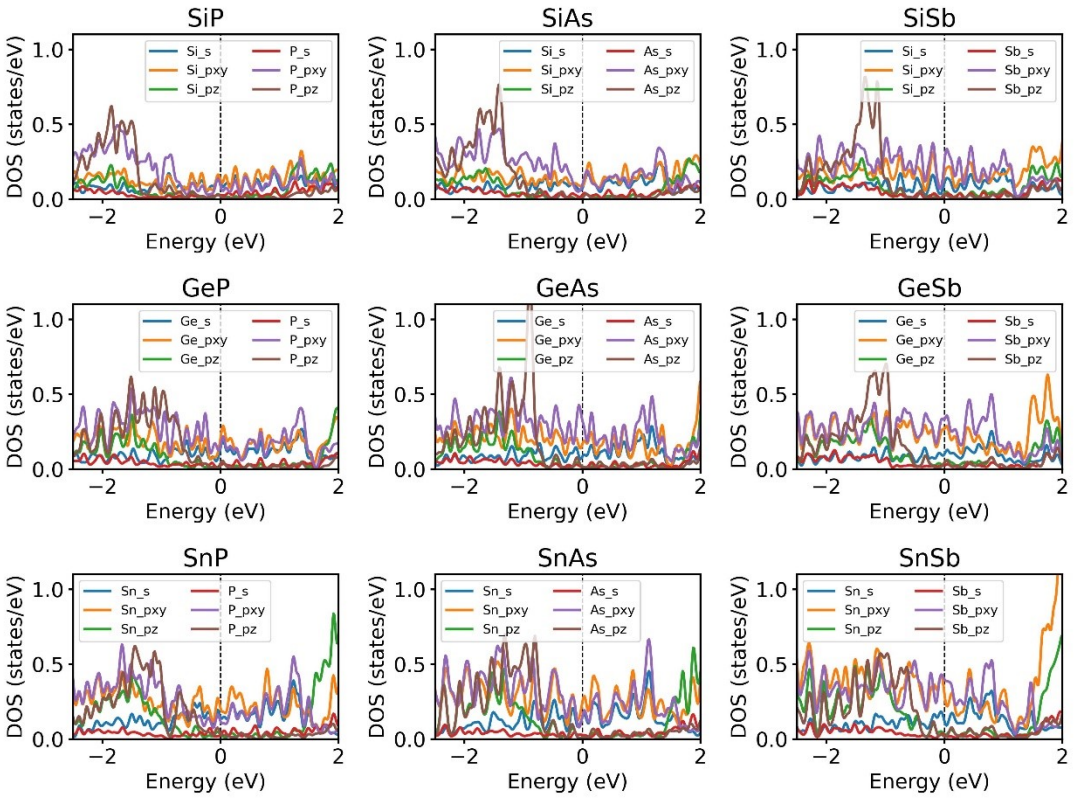

Fig. S2 The elemental- and orbital-resolved density of states (DOS) of group IV-V monolayers.

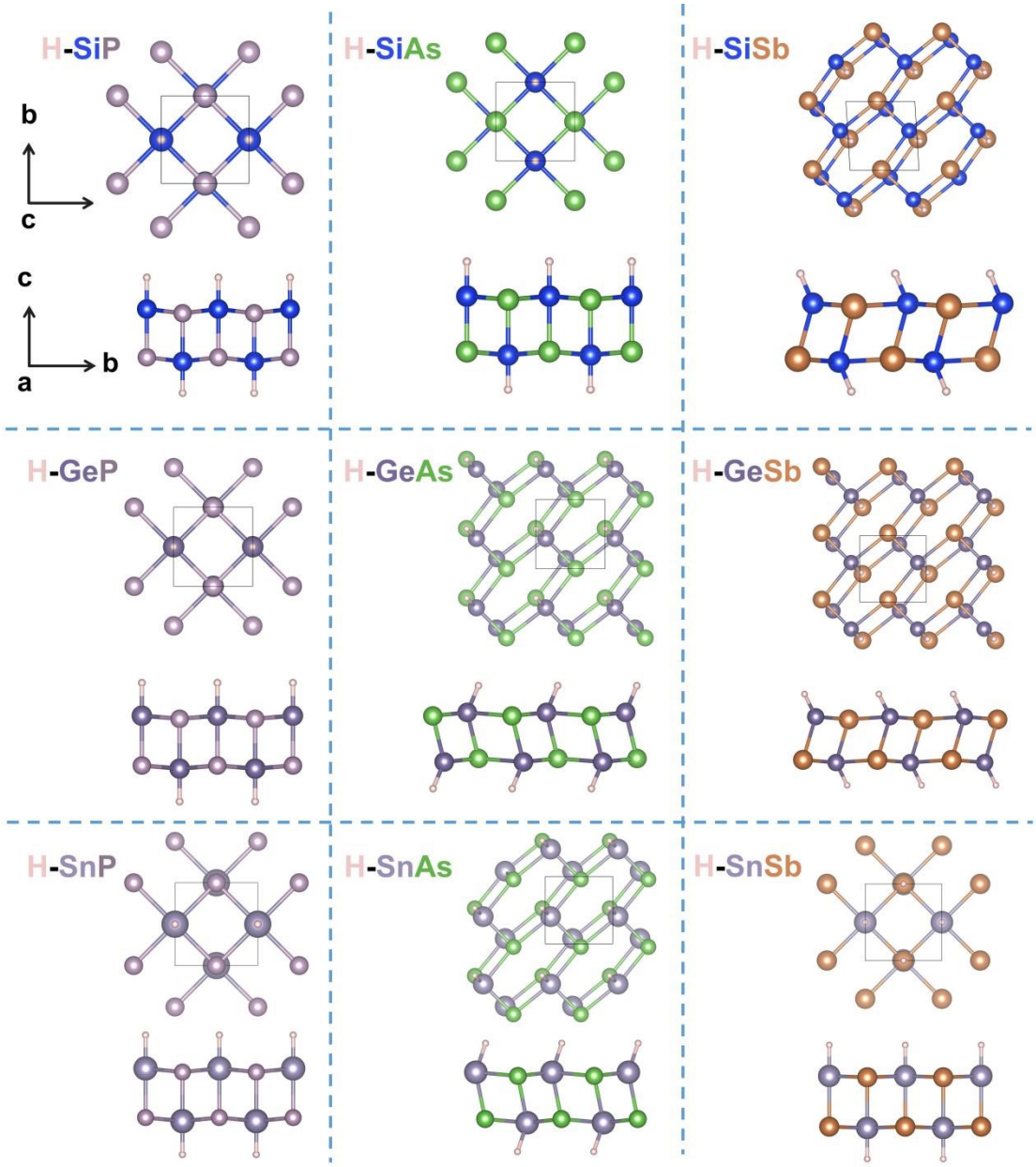

Fig. S3 Top and Side views of the optimized 2D hydrogenated group IV-V monolayers.

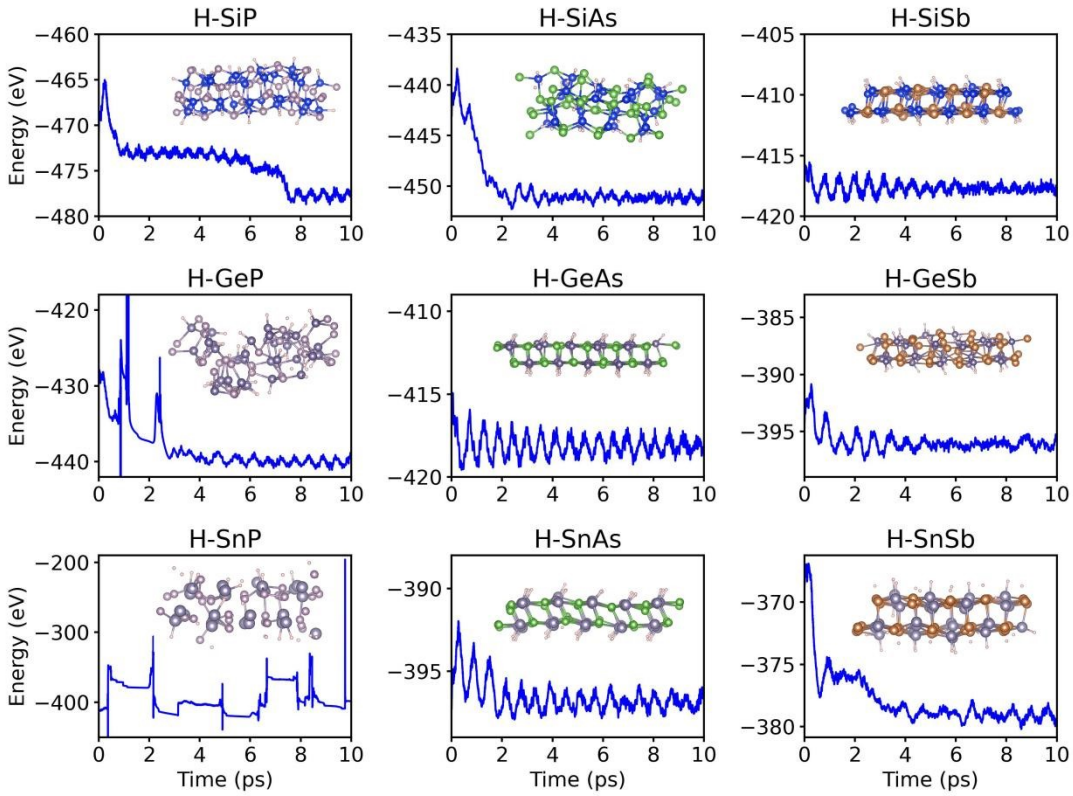

Fig.S4 The fluctuations of the total energy of 2D hydrogenated group IV-V monolayers during the AIMD simulations at 300K; the insets show the side views of the final structures at the end of the simulation.

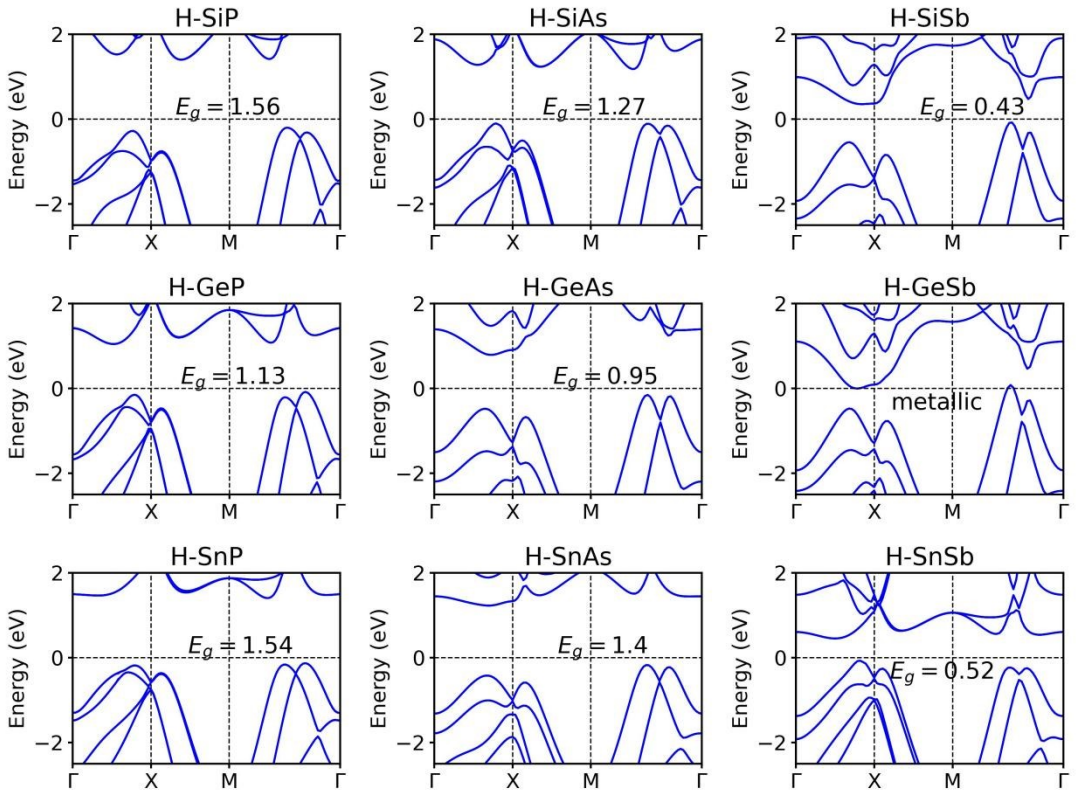

Fig. S5 Band structures of hydrogenated group IV-V monolayers in the Td4 structure calculated with the HSE functional with SOC.

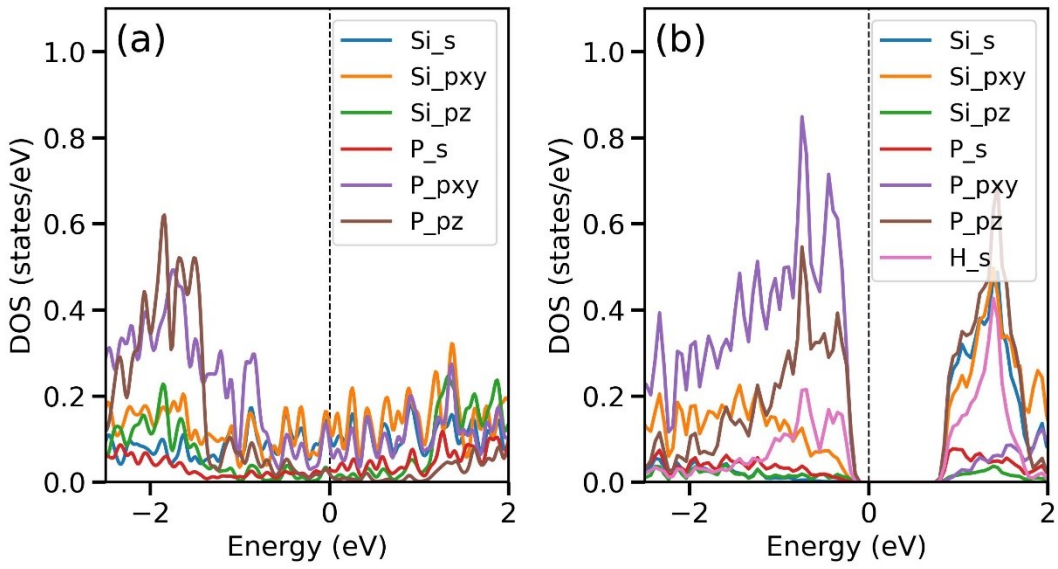

Fig. S6 The elemental- and orbital-resolved DOS of Td4-phase SiP monolayer and hydrogenated SiP monolayer.