Electronic Supplementary Material (ESI) for RSC Advances.

Supplemental Material for: Hydrogenated Derivatives of Hexacoordinated Metallic Monolayer Cu_2Si

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I. PHONON BAND STRUCTURES OF HYDROGENATED DERIVATIVES OF Cu_2Si WITH VARIOUS HYDROGEN CONCENTRATIONS

Geometries of several hydrogenated derivatives of Cu_2Si with different hydrogen concentrations are optimized. In order to analyze their dynamical stability, their phonon band structures are calculated. As it is seen from FIG. S1 and FIG. S2, these hydrogenated structures are found to be dynamically unstable since all of them include some negative frequency domains in their phonon branches.

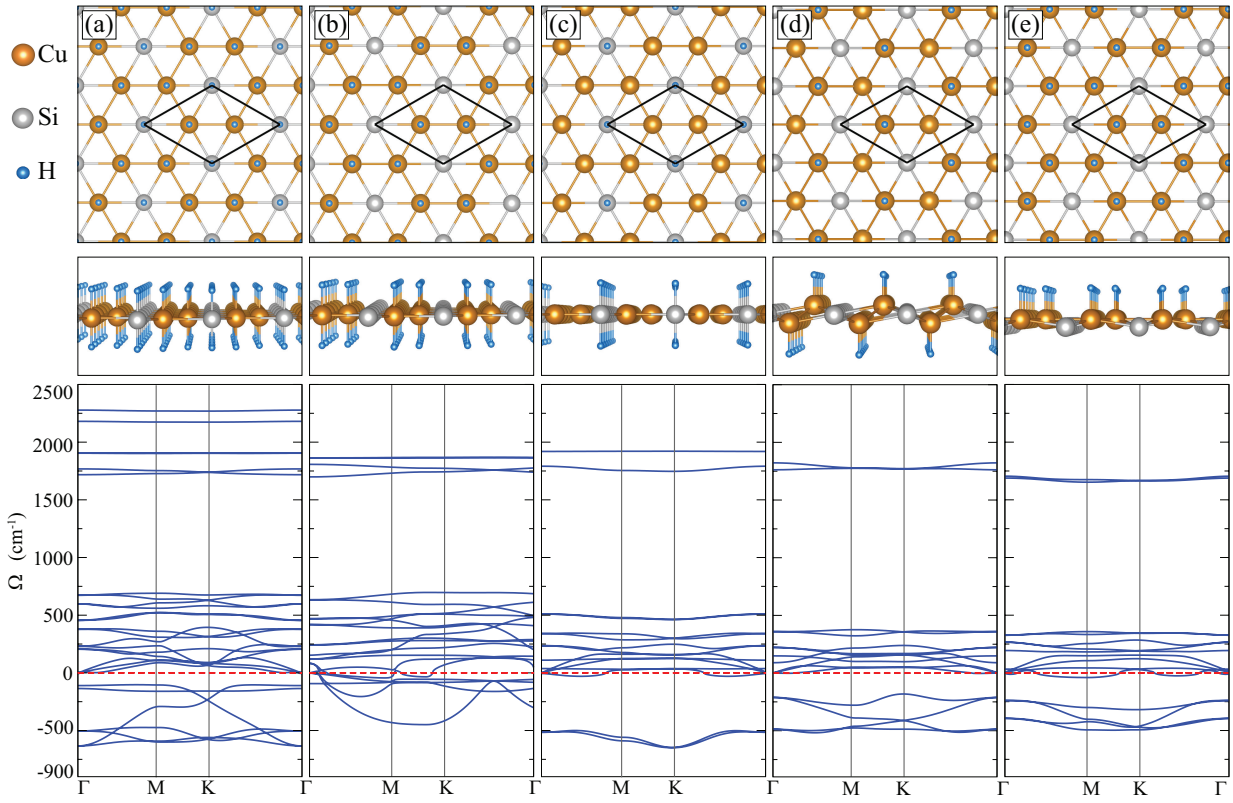

FIG. S1 (Color online) Optimized geometries and their calculated phonon band dispersion of several hydrogenated derivatives of monolayer Cu_2Si. Black rhombuses represent the unit cells.

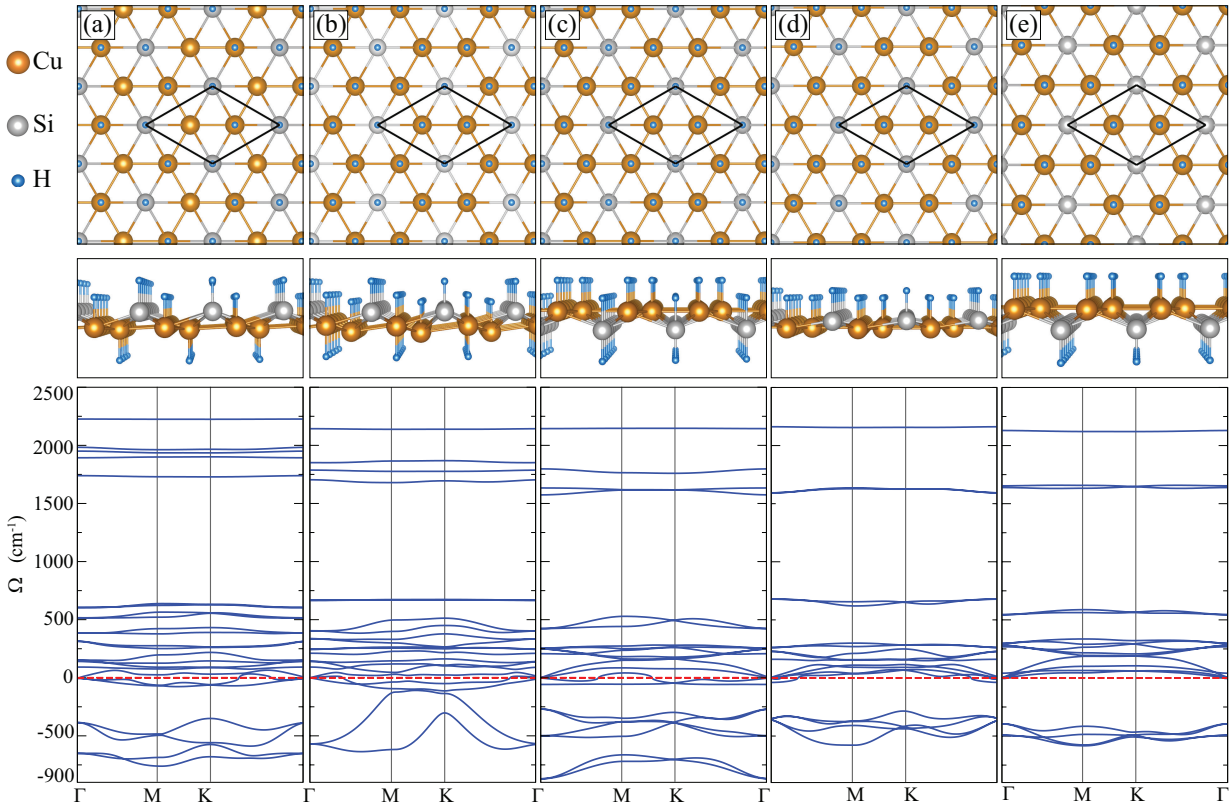

FIG. S2 (Color online) Same as FIG. S1