Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information for

"Hydrogenation-Induced Large-Gap Quantum-Spin-Hall Insulator States in Germanium-Tin Dumbbell Structure"

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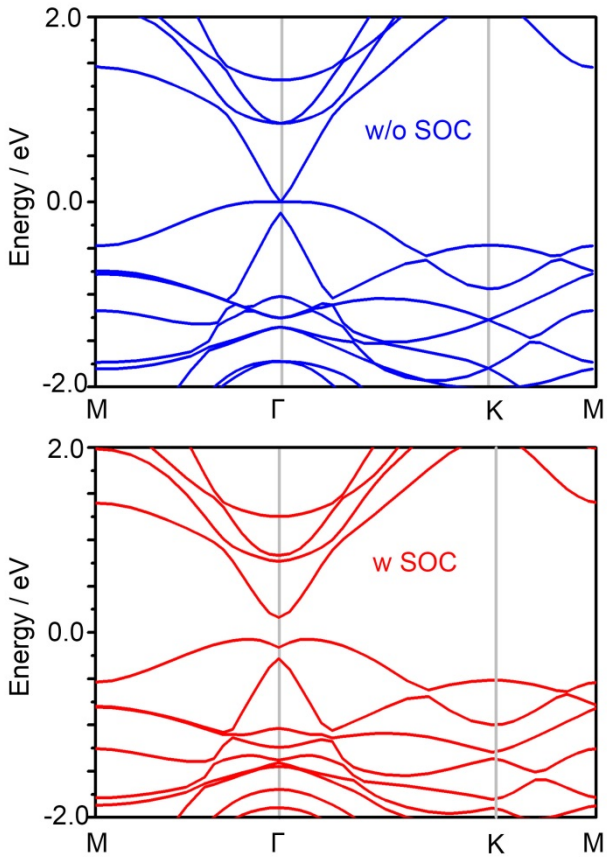

Figure S1. Electronic band structures of DB $Sn_6Ge_4H_4$without (up panel) and with (down panel) SOC obtained by using a hybrid functional in the form of Heyd–Scuseria–Ernzerhof (HSE). A small tensile strain (~2%) was applied to the lattice. The energy at the Fermi level was set to zero.

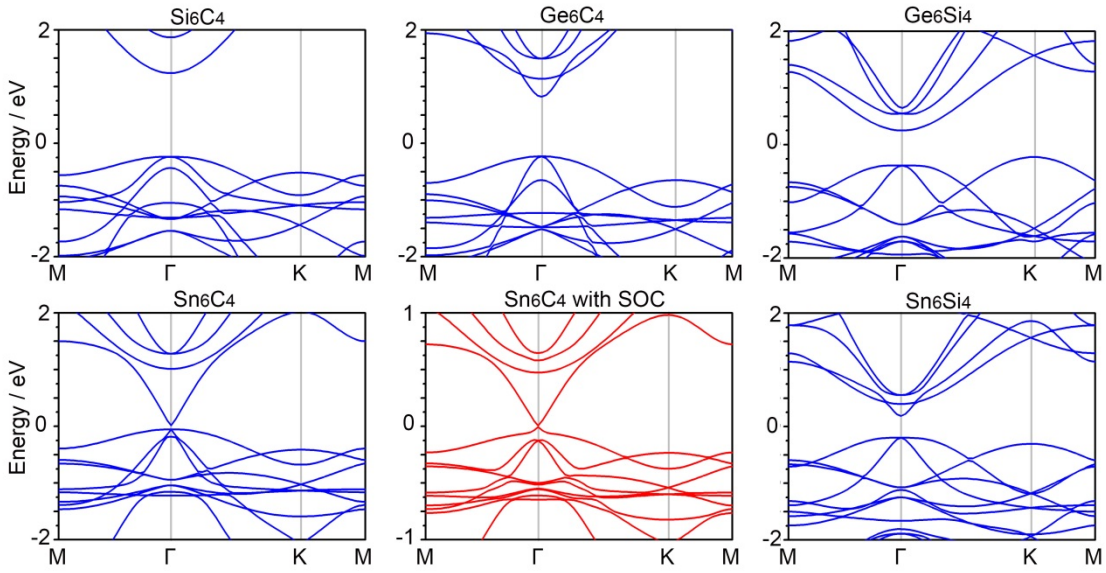

Figure S2. Electronic band structures of group-IV binary compounds with DB configurations.The blue lines indicate the bands without SOC. For DB Sn_6C_4, the band structure with SOC (the red lines) was plotted. Obviously, it is not a QSH insulator.

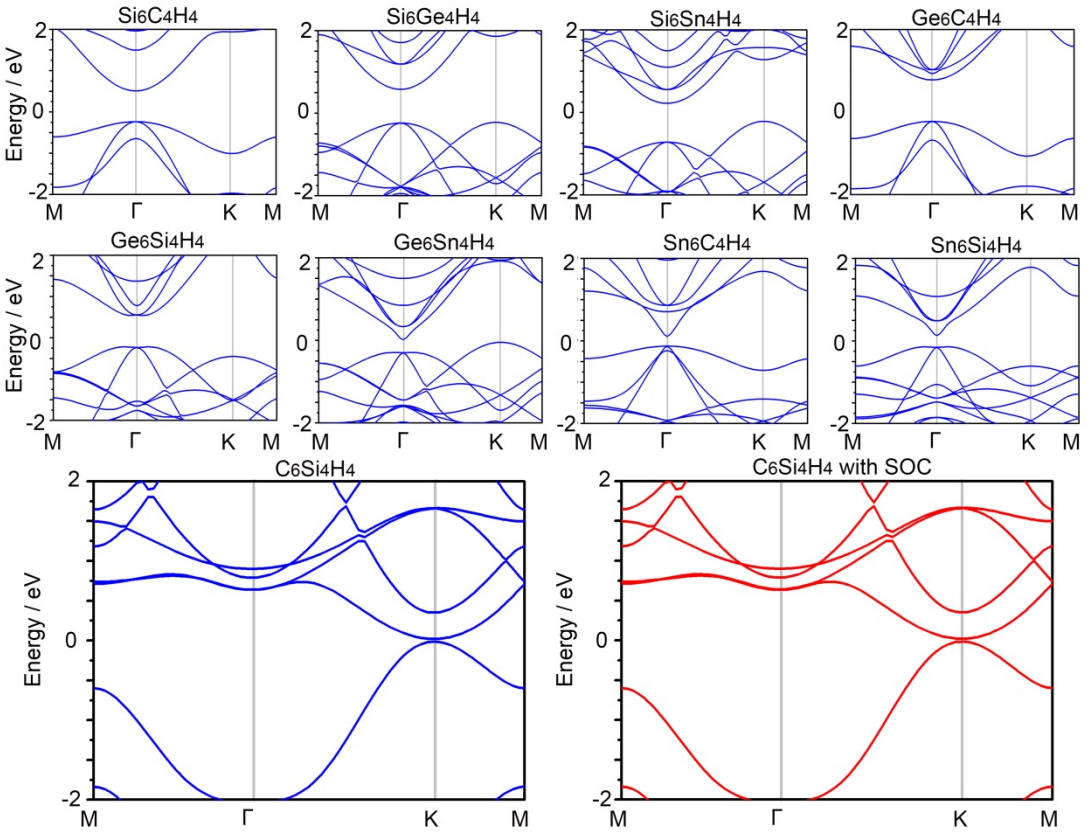

Figure S3. Electronic band structures of hydrogenated group-IV binary compounds with DB configurations.The blue lines indicate the bands without SOC. For DB $C_6Si_4H_4$, the band structure with SOC (the red lines) was plotted. Obviously, it is not a QSH insulator. Obviously, s-p band inversion doesn't take place in these band structures and none of them are QSH insulators.