Electronic Supplementary Information

Electronic structure of the ground and excited states of neutral and charged silicon hydrides, $SiH_x^{0/+/-}$, x=1−4

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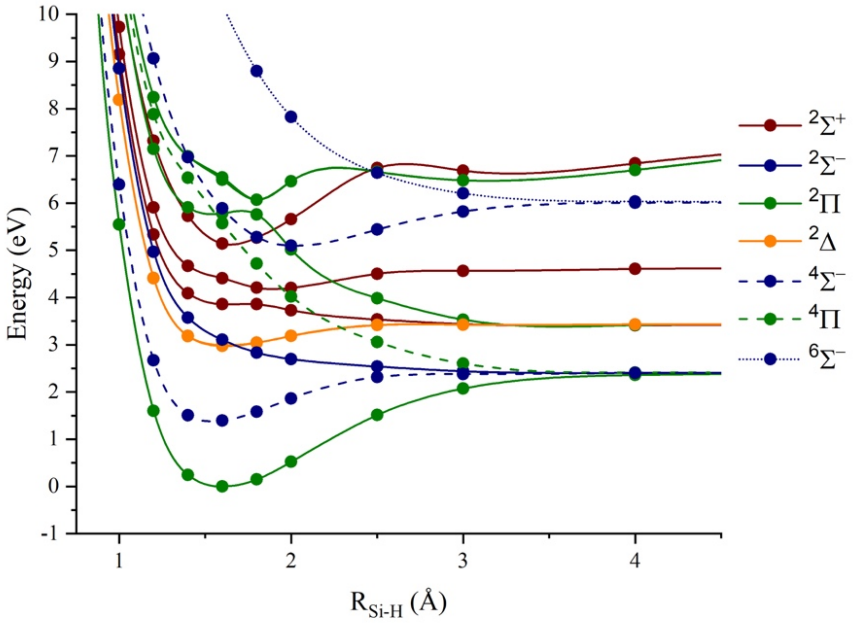

Figure S1. CASSCF potential energy curves for the low-lying states of SiH.

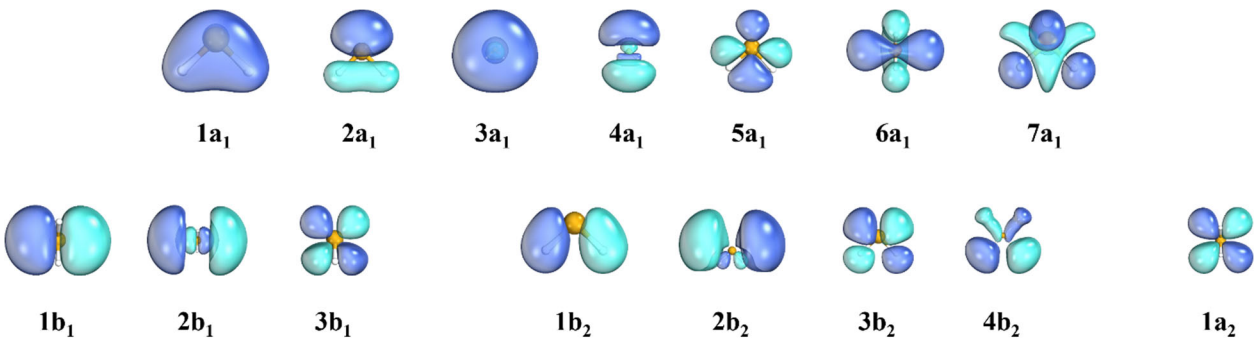

Figure S2. CASSCF active molecular orbitals of SiH_2.

Table S1. SiH bond lengths r_e (Å) and HSiH angles φ (degrees) for $SiH_3^{0,\pm}$ at CAM-B3LYP, MP2, and CCSD(T) levels of theory using aug-cc-pVTZ basis sets.

	r_e			φ		
Species	MP2	CAM-B3LYP	CCSD(T)	MP2	CAM-B3LYP	CCSD(T)
SiH_3^+	1.462	1.467	1.468	120.0	120.0	120.0
SiH_3	1.478	1.481	1.484	111.2	111.1	111.2
SiH_3^-	1.535	1.538	1.544	95.5	95.3	95.2