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The crystal structure and SiH_4-H_2 interactions of high-pressure $SiH_4(H_2)_2$ from first principles KYLE MICHEL, YONGDUO LIU, VIDVUDS OZOLINS, University of California, Los Angeles — Mixtures of SiH_4 and H_2 have recently been found to crystallize at pressures above 6.8 GPa. Here, the crystal structure, bonding, and vibrational properties of $SiH_4(H_2)_2$ over a range of applied pressures are studied using first-principles density functional theory (DFT) calculations. Results show a decrease in the frequencies of the intramolecular H_2 stretching modes with increasing pressure, contrary to the behavior of bulk H_2 under an applied pressure. This softening of the H_2 bond is found to be much more prominent for H_2 located in tetrahedral sites rather than in octahedral sites. DFT calculations suggest that the behavior of the H_2 bond is explained by an increased orbital overlap and electron sharing between silane and hydrogen molecules.

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