Anharmonicity in the vibrational modes associated with H-H, N-H, O-H, and C-H bonds

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Abstract: The anharmonic contributions to the vibrational frequency of various H-H, N-H, O-H, and C-H bond configurations are investigated using first principles calculations. While harmonic approximation can be accurately used to calculate the local vibrational mode of most microscopic configurations, the configurations involving strong X-H bond are exceptions because of the exceptionally light mass of the H atom. We will explicitly present the magnitude of the anharmonic contributions to the total frequencies associated with X-H bonds in free molecules as well as in semiconductors defects.

Ei controlled terms: **Hydrogen bonds** - Semiconductor materials - Vibration measurement - Infrared spectroscopy - Gallium nitride - Oscillistors - Absorption