Density Functional Theory Study of the Si2h6-Xfx Series of Molecules

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Abstract

The systematic replacement of hydrogen by fluorine atoms in disilane (Si2H6) is investigated using density functional theory (DFT). For every molecule in the Si2H6xFx family, with 0 6 x 6 6, we find the energetically most favorable configurations. Properties such as chemical potential, chemical hardness, polarizability, electrophilicity and the infrared vibration modes and frequencies are evaluated and analyzed in terms of the fluorine substitution. The molecular response to twisting the silyl groups at each end of the Si–Si axis, relative to each other, is also investigated. A consistent picture emerges which is in good agreement with the available experimental results.