Electronic Properties of Disilane: An ab initio Calculation

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Abstract

We calculate from first principles the electronic ground and excited state, geometrical and vibrational properties of the staggered and eclipsed disilane (Si2H6) conformations. We find that, due to the rotation of a silyl group around the Si–Si axis, significant changes of the physical properties are induced. Therefore, depending on the conformation, the reactivity of disilane may be strongly altered.