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Electronic Structure of Optimized Si_mH_n Clusters: MINDO3 and AM1 Calculations

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Abstract: We have investigated the electronic structure of optimized hydrogenated silicon microclusters. Si_mH_n (m=2,3,5,6; n = 4,6) have been investigated. The calculations were performed using both MINDO3 and AM1 semiempirical molecular orbital methods.

Key Words: Electronic structure, clusters, semiempirical methods

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