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Electronic structure and thermochemistry of Si_n clusters(n=2-11)

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Abstract: *Agglomerates and nanostructured materials containing a few atoms (in the order of magnitude of 10^0-10^2 units) present potential in the development of new materials in several technological areas crucial for human society in the 21st century, such as electronics*[1–3], *catalysis, chemical resistors and X-rays. Due to their low dimensionality, these clusters make it possible to create new routes for some processes and increase the efficiency of devices*[1,2]. *Also, the miniaturization of electronic components in processors crossed the line between the microscopic systems governed by classical mechanics and sub-microscopic systems governed by quantum mechanics. In 2016, commercial transistor processing technology is 14 nm*[4], *that is, on the order of 100 atoms in length, with 10 nm transistors expected to be produced on an industrial scale by 2018. On a laboratory scale, transistors with technology of 7 nm are under development.*

In this work, we focused in characterize the "magic numbers" of Si_n (n=2-11) series through DFT method within M06 approximation combined with 6-311++G(3df,3pd) atomic basis set. The stability analysis was carried out with the Hartree-Fock orbitals energy diagram and on the atomization Free Gibbs Energy and atomization Enthalpy evaluation. The results obtained in the present work, shows Si_6 and Si_{10} as "magic numbers" in agreement with previously theoretical and experimental works.

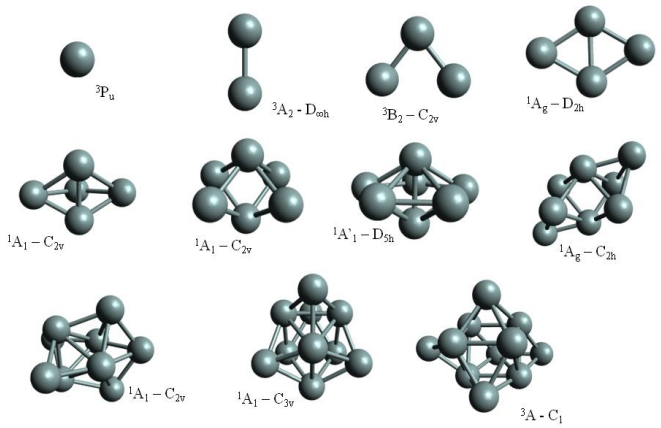

Figure 1. Growth pattern of the Si_n clusters, n=1-11, through the M06/6-311++G(3df,3pd) methodology.

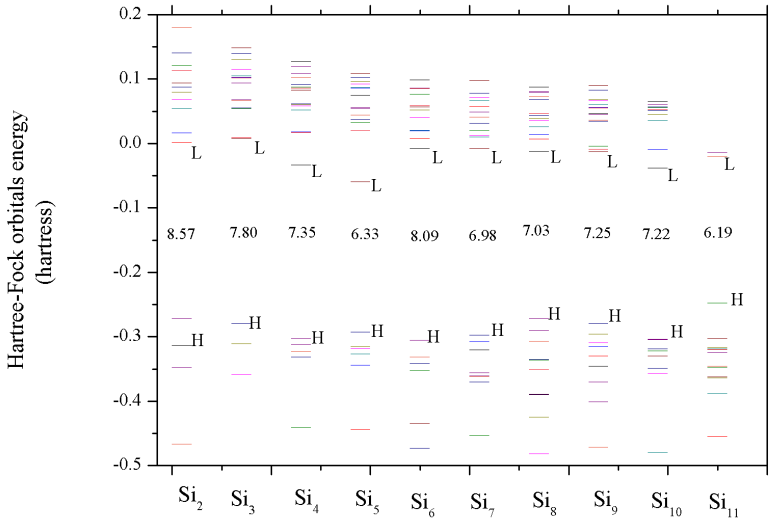

Figure 2. Hartree-Fock orbitals energy diagram of the Si_n clusters, n=2 - 11, through the HF/6-311++G(3df,3pd) methodology.

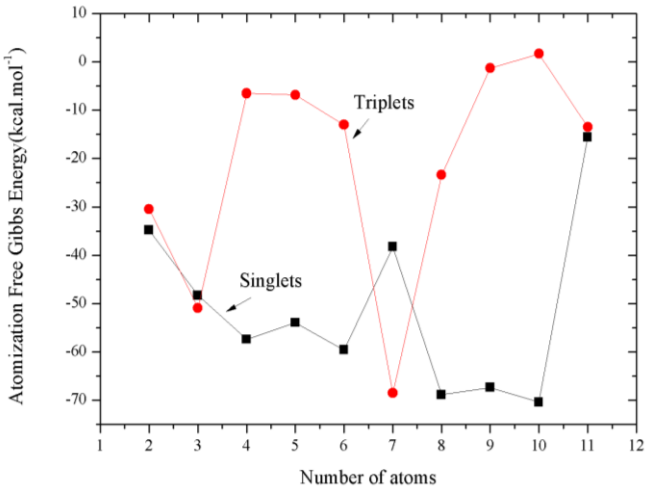

Figure 3. Atomization Free Gibbs Energy of the Si_n clusters at singlet and triplet spin multiplicity, n=2 - 11, through the M06/6-311++G(3df,3pd) methodology.

Key-words: *nanomaterials, electronic structure, thermochemistry, silicon clusters.*
Support: *ITA*

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