

Supplementary Information:

Mn₂@Si₁₅: the smallest triple ring tubular silicon cluster

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This file contains:

- Comparison of the shapes of core s-MOs set of Mn₂Si₁₅ produced by DFT calculations with the wavefunctions obtained by the hollow cylinder model.
- Comparison of the shapes of radial r-MOs set of Mn₂Si₁₅ produced by DFT calculations with the wavefunctions obtained by the hollow cylinder model.
- Comparison of the shapes of tangential t-MOs set of Mn₂Si₁₅ produced by DFT calculations with the wavefunctions obtained by the hollow cylinder model.

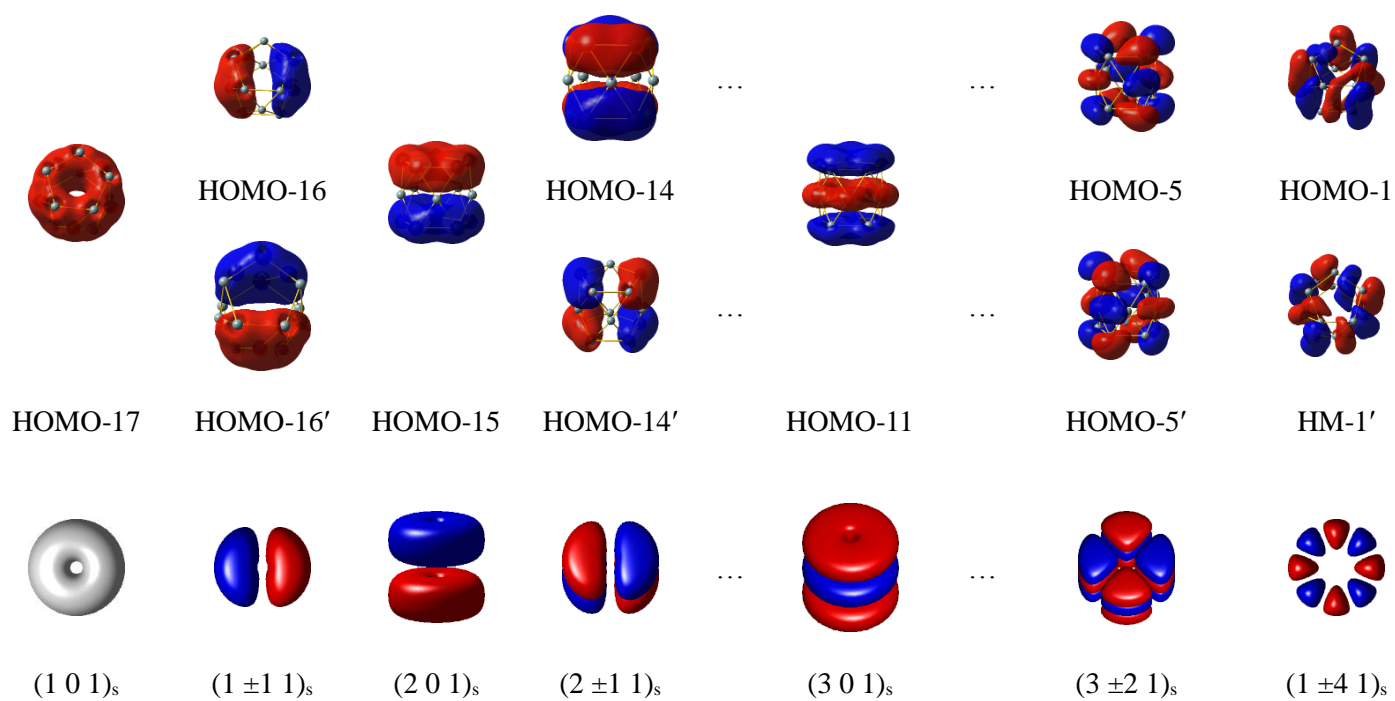


Figure S2. Some shapes of s-MOs of Si₁₅ triple ring computed using DFT/BP86/6-311+G(d) and the corresponding wave function obtained by solving the Schrödinger equation for a particle in a hollow cylinder model.

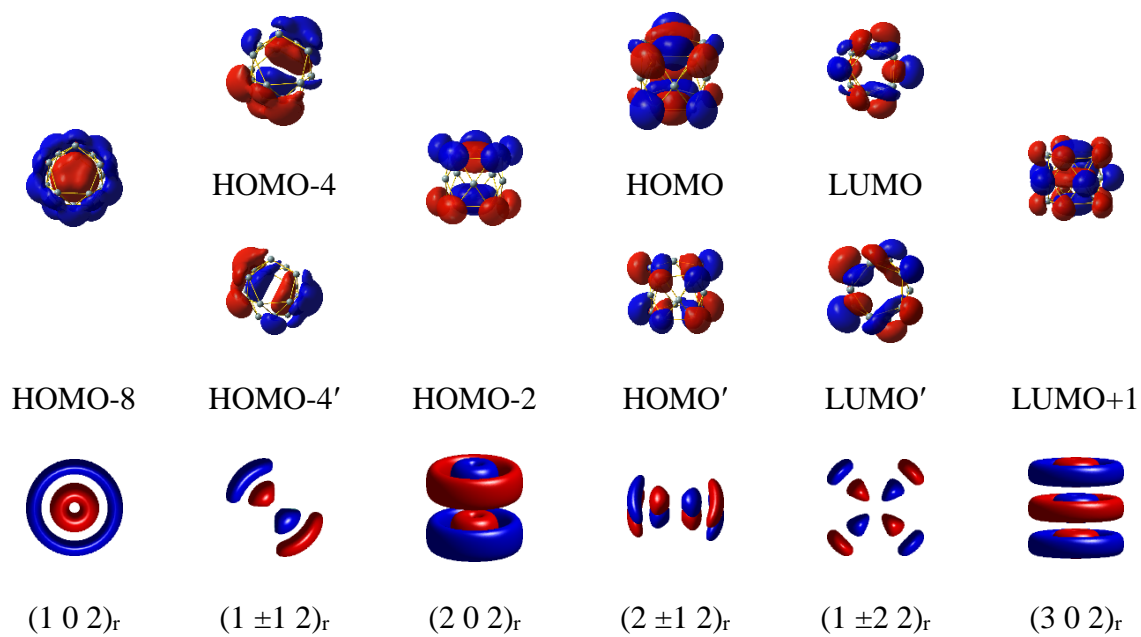


Figure S3. Shapes of r-MOs of Si₁₅ triple ring computed using bp86/6-311+G(d) and the corresponding wave function obtained by solving the Schrödinger equation for the particle in a hollow cylinder model.

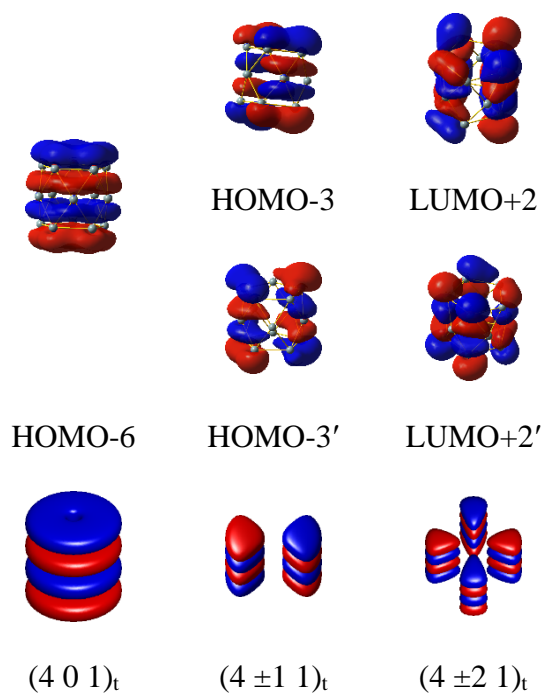


Figure S4. Shapes of t-MOs of Si₁₅ triple ring computed using DFT/BP86/6-311+G(d) and the corresponding wave function obtained by solving the Schrödinger equation for the particle in a hollow cylinder model.