Abstract Submitted
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The Lowest Energy Structures of Si-24 Cluster[1] J. RUFINUS, Widener University — We present the results of computational calculations of the lowest energy structures of Silicon 24 cluster. The calculations were done in the framework of DFT with PBE exchange functional. The initial structures were calculated using a Genetic Algorithm. Approximately 1000 structures were recalculated using Gaussian 03 (with the basis set 6-31G) to determine the lowest energy structures.

[1]The computations were performed in part on the NSF Terascale Computing System at the Pittsburgh Supercomputing Center.

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