

Machine-learning enhanced global search for medium-size silicon clusters: new minima for Si₁₈, Si₂₀, Si₃₀, and Si₃₂

Electronic Supplementary Information

Jesús Iván Salazar-Barrientos^a, Clare McCabe^b, Peter T. Cummings^b, Tomás Rocha-Rinza^a,
José Manuel Guevara-Vela^{b,*}

^a*Instituto de Química, Universidad Nacional Autónoma de México, Circuito Exterior, Ciudad Universitaria, Delegación Coyoacán C.P. 04510, Ciudad de México, Mexico.*

^b*School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh EH14 4AS, Scotland, U.K.*

1. Associated files

The data associated with this work are available at

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The repository contains the Cartesian coordinates of the silicon cluster structures discussed in this study, including the newly identified low-energy structures and the corresponding reference structures from the literature. The trained NequIP models and the underlying training data used to construct the MLIPs are also provided to facilitate reproducibility and further benchmarking.

*To whom correspondence should be addressed: j.guevara-vela@hw.ac.uk

2. Relative Gibbs free energies at 298 K

Table S1: Relative Gibbs free energies at 298 K, ΔG_{298} , of selected Si_n structures with respect to the lowest-energy structure identified for each cluster size. The ΔG_{298} values include zero-point and thermal corrections. Values are given in kcal mol^{-1} . The geometries and thermal/ZPE corrections were obtained at the PBE0/def2-TZVP level, whereas the electronic energies were evaluated at the DLPNO-CCSD(T)/cc-pVTZ level. The columns correspond to structures from the QCD database of Manna et al.^[1], the structures reported by Yoo et al.^[2], and the structures identified in this work.

Cluster	QCD	Yoo et al.	This work
Si_{18}	10.6	4.2	0.0
Si_{20}	9.4	—	0.0
Si_{30}	22.4	2.7	0.0
Si_{32}	13.2	8.0	0.0

3. Principal moments of inertia

Table S2: Principal moments of inertia of the newly identified low-energy structures. The moments are sorted as $I_a \leq I_b \leq I_c$ and were used to compute the triaxiality parameter T and asphericity A reported in the main text.

Cluster	I_a	I_b	I_c
Si ₁₈	1881.476	4051.794	4135.865
Si ₂₀	2281.089	5048.265	5293.215
Si ₃₀	6134.961	6940.905	7783.877
Si ₃₂	7418.980	7769.483	8189.983

References

- [1] S. Manna, Y. Wang, A. Hernandez, P. Lile, S. Liu, T. Mueller, *Sci. Data* **2023**, *10*, 308.
- [2] S. Yoo, X. C. Zeng, *Angew. Chem. Int. Ed.* **2005**, *44*, 1491–1494.