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Data Article

Systematic and efficient navigating potential energy surface: Data for silver doped gold clusters

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ABSTRACT

Locating global minimum of certain atomistic ensemble is known to be a highly challenging and resource consuming task. This dataset represents joint usage of the semi-empirical PM7 Hamiltonian, Broyden–Fletcher–Goldfarb–Shanno algorithm and basin hopping scheme to navigate a potential energy surface. The Au_{20} nanocluster was used for calibration as its global minimum structure is well-known. Furthermore, $Au_{18}Ag_2$ and $Au_{15}Ag_5$ were simulated for illustration of the algorithm performance. The work shows encouraging results and, particularly, underlines proper accuracy of PM7 as applied to this type of heavy metal systems. The reported dataset motivates to use the benchmarked method for studying potential energy surfaces of manifold systems and locate their global-minimum atomistic configurations.

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Specification Table

Subject area	*Physics*, *Chemistry*
More specific subject area	*Computational Molecular Science*
Type of data	*Tables, figures*
How data was acquired	*Computer simulation*
Data format	*Filtered*, *analyzed*

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Experimental factors	*Computer simulations at the Neumann supercomputing cluster*
Experimental features	*Computer simulations at the Neumann supercomputing cluster*
Data source location	*São Paulo, Brazil*
Data accessibility	*All data are in this article*

Value of the data

- Since accuracy of PM7 was proven for gold nanoclusters, this method can be applied to other important problems in materials chemistry.
- Knowledge regarding low-energy local minima of gold nanoclusters is useful to develop future synthetic methods and identify experimental structures.
- The reported geometries and formation energies for unusual conformers can be elaborated using higher-level methods in computational chemistry.

1. Data

The paper reports possible local-minima structures of Au_{20}, $Au_{18}Ag_2$, $Au_{15}Ag_5$ obtained from the potential energy surface scans. Starting from an arbitrary geometry, a correct structure of the Au_{20} nanocluster will be found (an experimental global-minimum conformation of Au_{20} is known to be a pyramid with the T_d point group symmetry) [1].

2. Experimental design, materials and methods

The wave functions of the GNCs at every optimization step were represented by means of the PM7 semi-empirical Hamiltonian [2]. PM7 uses the approximation of neglect of diatomic differential overlap, as applied to the Hartree–Fock (HF) method. In turn, all terms of the exact Hamiltonian in HF are expressed as a sum of one-electron operators. Unlike in HF, selected integrals in PM7 are parametrized in view of empirical data and may potentially provide more accurate results than HF. The convergence criterion of the wave function was set to 4.18×10^{-4} kJ mol^{-1}(Figs. 1–8).

The local optimizations were done by means of the Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm [3]. This algorithm is essentially failure-proof at the expense of a significant number of iterations (single-point calculations) before it converges. The geometry convergence criterion was set to 1.0 kJ mol^{-1} Å^{-1}, which systematically corresponds to less than 0.1 kJ mol^{-1} difference in total energy at two consequent BFGS steps (Table 1).

The global optimization was propagated in the framework of the basin hopping (BH) algorithm [4]. Fifty one iterations were performed for every system and the resulting energies were compared to one another. The maximum displacement per gold atom was allowed to be 0.75 Å whereas effective temperature was set to 2000 K. The effective temperature is used to accept or decline possible translations/perturbations within the Metropolis test. For an efficient search, the temperature must be comparable to the higher barrier separating local minima on PES. Since different conformations of GNCs involve different order of bonds between the gold atoms, the bond breakage is required to go from one stable conformation towards another. The effective temperature parameter must be significantly large for the above reason.

The in-home code for navigating PES makes use of the implemented optimization routines provided by SciPy and ASE with minor technical modifications [5]. Implementation of PM7 in MOPAC2012 (openMOPAC.net), as provided by Dr. J.J.P. Stewart, was used. All structures and optimization pathways were visualized in VMD, version 1.9.1 [6]. Input structures were prepared in Gabedit [7].

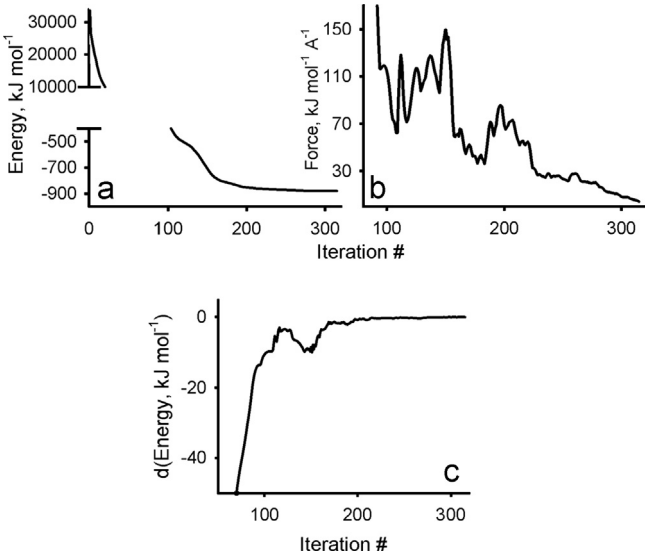

Fig. 1. Geometry optimization of the silver doped gold nanoclusters. The minimized formation heat corresponds to local minimum structures.

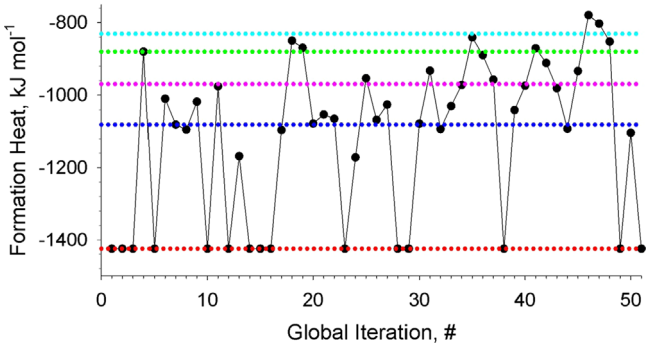

Fig. 2. Formation energies of the revealed local-minimum structures of Au_{20}. The dotted color lines depict energies of the structures, which were obtained most frequently.

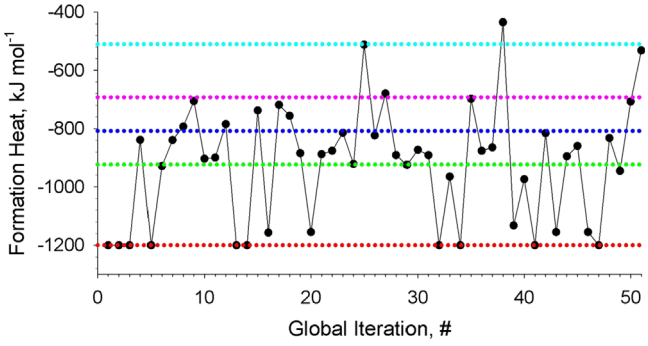

Fig. 3. Formation energies of the revealed local-minimum structures of $Au_{18}Ag_2$. The dotted color lines depict energies of the structures, which were obtained most frequently.

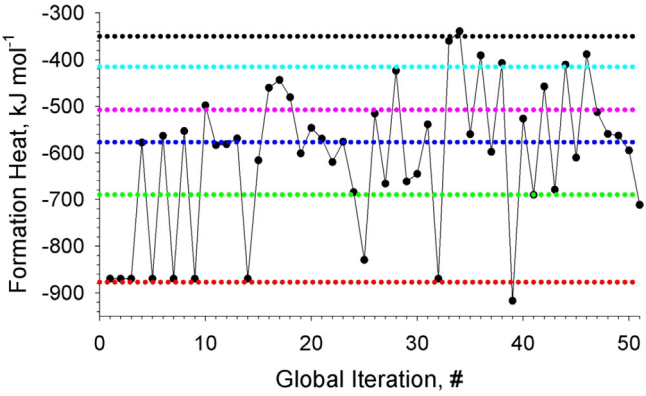

Fig. 4. Formation energies of the revealed local-minimum structures of $Au_{15}Ag_5$. The dotted color lines depict energies of the structures, which were obtained most frequently.

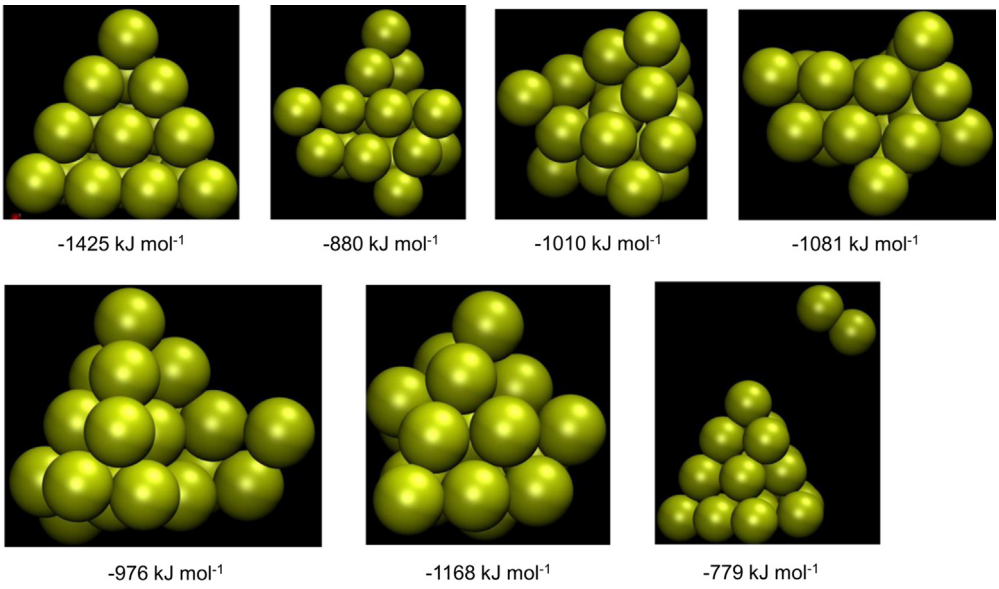

Fig. 5. Representative stable structures of Au_{20} and corresponding formation energies.

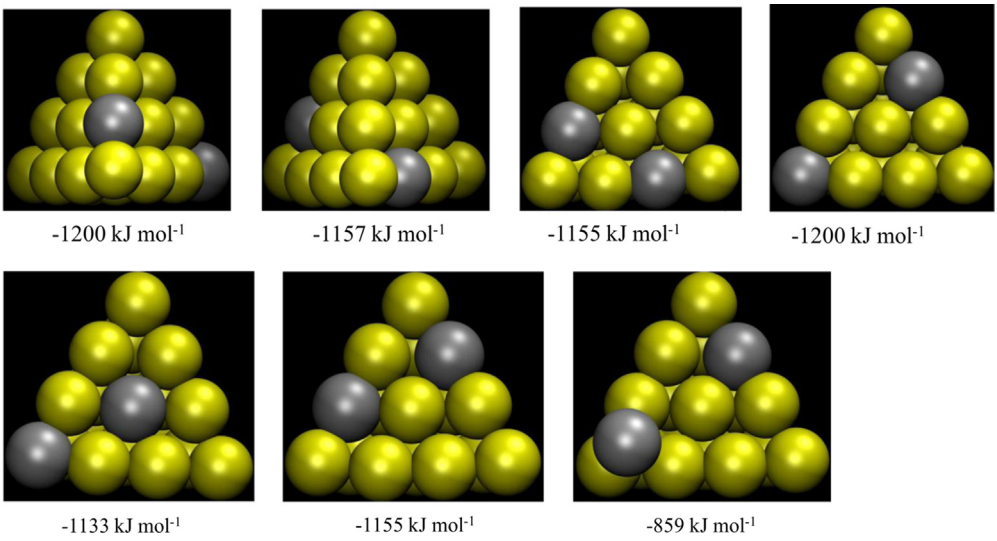

Fig. 6. Representative stable structures of $Au_{18}Ag_2$ and corresponding formation energies.

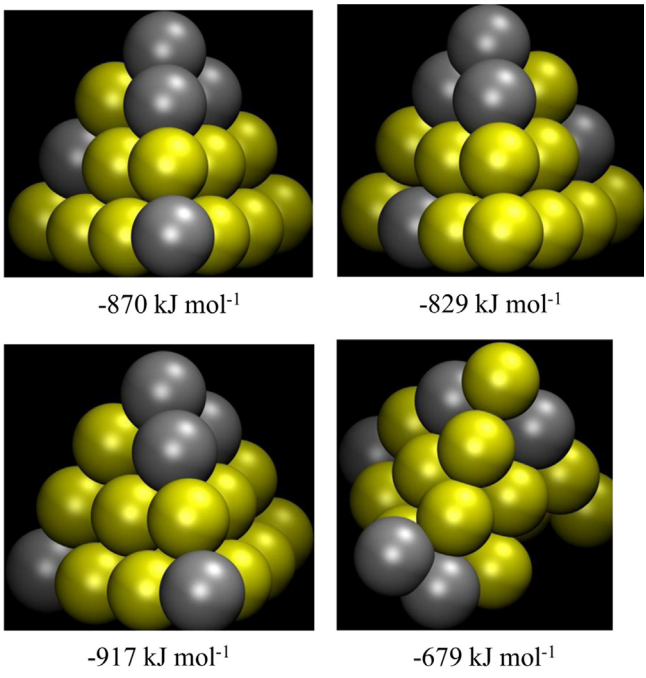

Fig. 7. Representative stable structures of $Au_{15}Ag_5$ and corresponding formation energies.

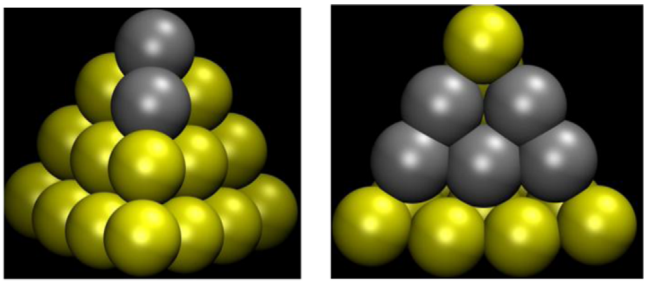

Fig. 8. Local-minimum structures and formation energies of $Au_{18}Ag_2$ and $Au_{15}Ag_5$ with maximum number of chemical bonds between silver atoms.

Table 1
Technical details of global minimum search: total number of electrons in each system; number of electrons simulated implicitly; total number of single-point computations (SPCs) performed; the largest number of SPC iterations per one geometry optimization.

Cluster	Total electrons	Implicit electrons	Total number of SPCs	Largest number of SPCs per local optimization
Au_{20}	1580	1360	35,350	4611
$Au_{18}Ag_2$	1516	1296	19,150	742
$Au_{15}Ag_5$	1420	1200	32,267	3025

Acknowledgments

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Appendix A. Supplementary material

Supplementary data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2016.04.014.

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