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Evidence of hollow golden cages: Supplementary Materials and Supporting Information

Satya S. Bulusu

University of Nebraska-Lincoln, sbulusu@iiti.ac.in

Xi Li

Rowland Institute at Harvard, li@rowland.harvard.edu

Lai-Sheng Wang

Washington State University & Pacific Northwest National Laboratory, ls.wang@pnl.gov

Xiao Cheng Zeng

University of Nebraska-Lincoln, xzeng1@unl.edu

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Supplementary Materials for

Evidence of hollow golden cages

Satya Bulusu*, Xi Li^{†‡§}, Lai-Sheng Wang^{†‡¶}, and Xiao Cheng Zeng*[¶]

* Department of Chemistry and Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE 68588;

† Department of Physics, Washington State University, 2710 University Drive, Richland, WA 99354; and

‡ Chemical Sciences Division, Pacific Northwest National Laboratory, MS K8-88, P.O. Box 999, Richland, WA 99352

¶ To whom correspondence may be addressed. E-mail: ls.wang@pnl.gov or xczeng@phase2.unl.edu

§ Present address: Rowland Institute at Harvard, 100 Edwin H. Land Boulevard, Cambridge, MA 02142

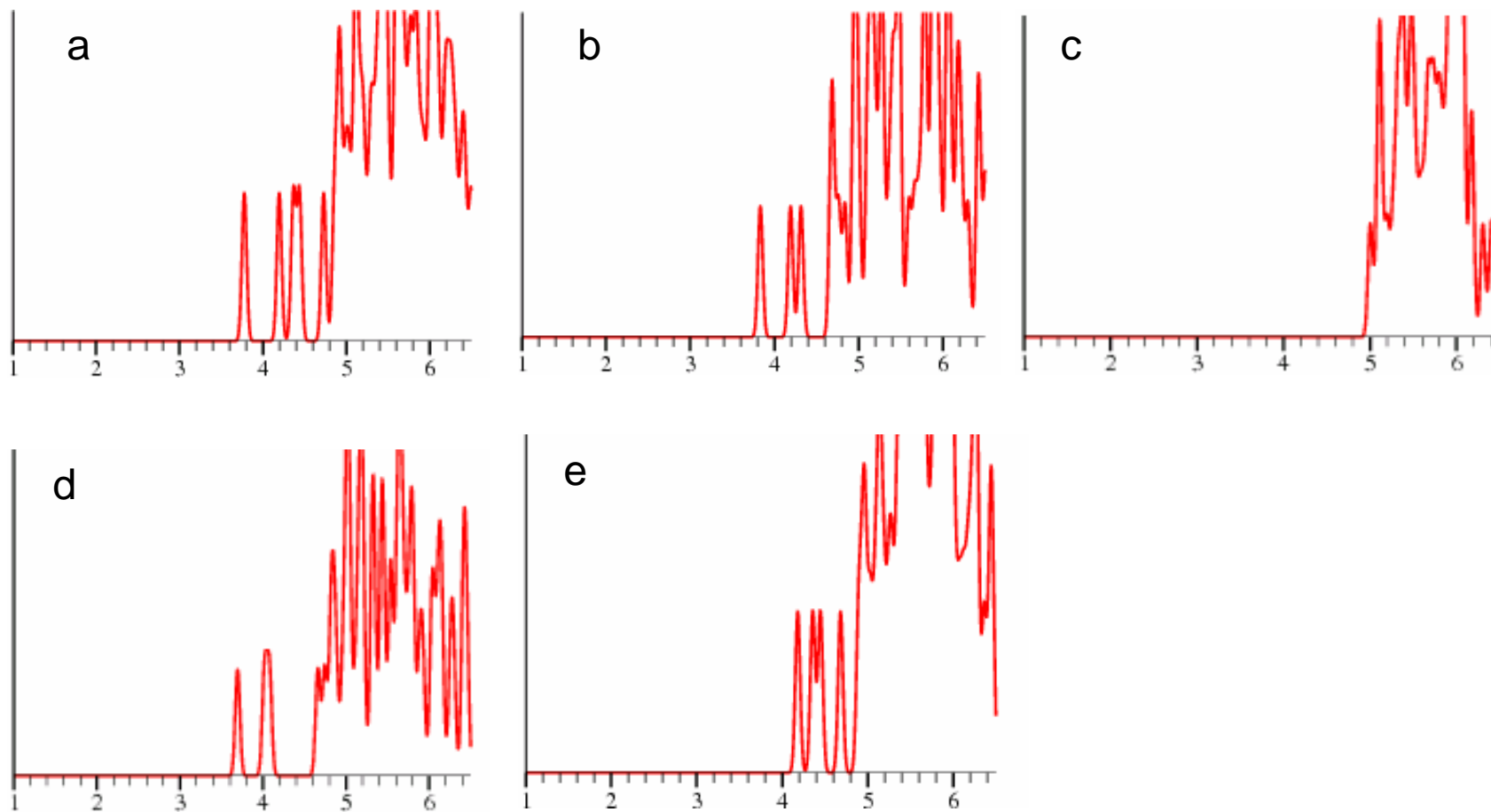
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Fig. 3. Simulated anion photoelectron spectra [based on the density-functional theory (DFT) calculation with the PBEPBE/LANL2DZ functional and basis set] for all of the candidate lowest-energy isomers of Au₁₅⁻ (A), Au₁₆⁻ (B), Au₁₇⁻ (C), and Au₁₈⁻ (D) identified in Fig. 3 A–D, respectively.

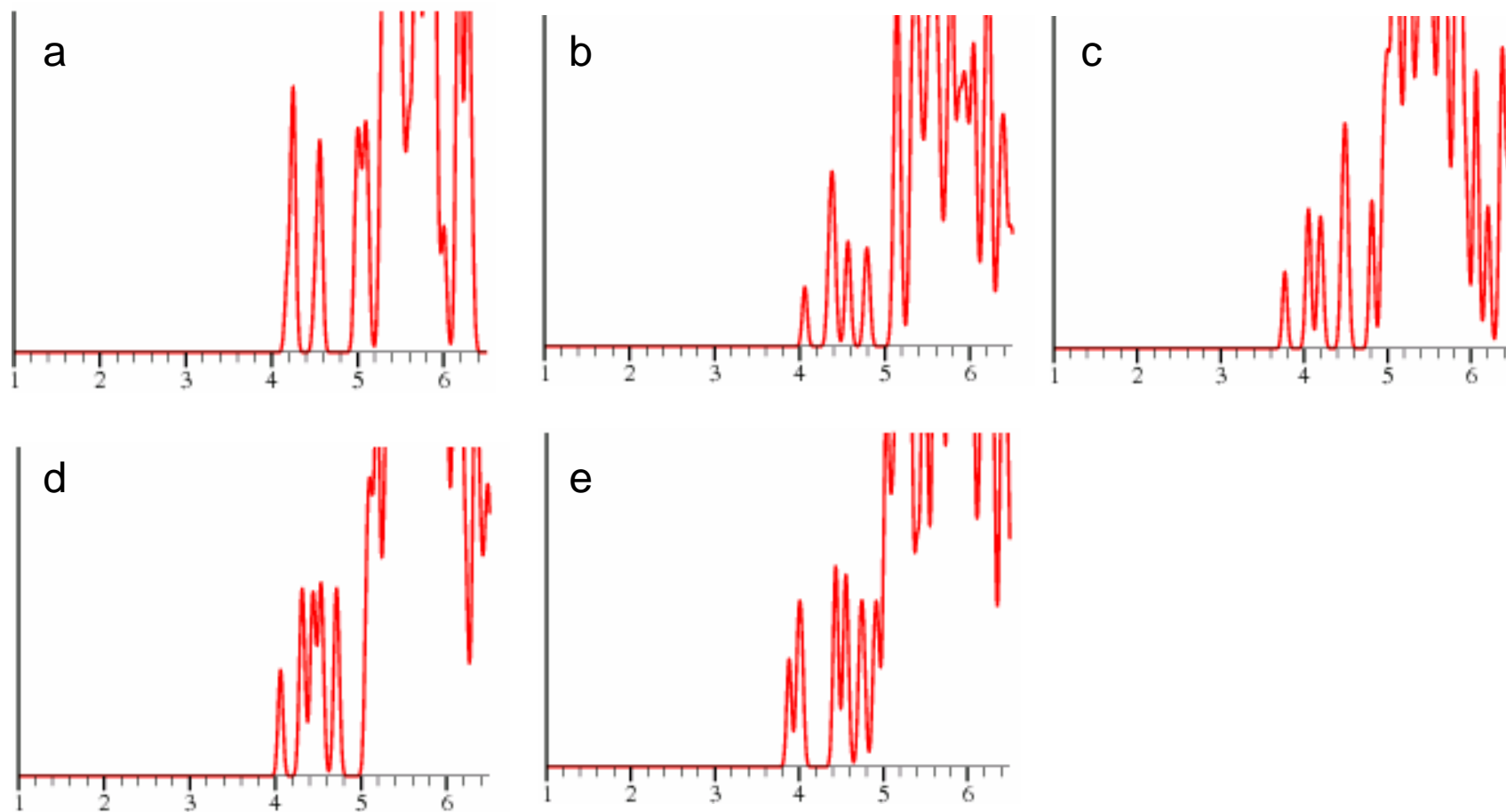
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Simulated Anion Photoelectron Spectra



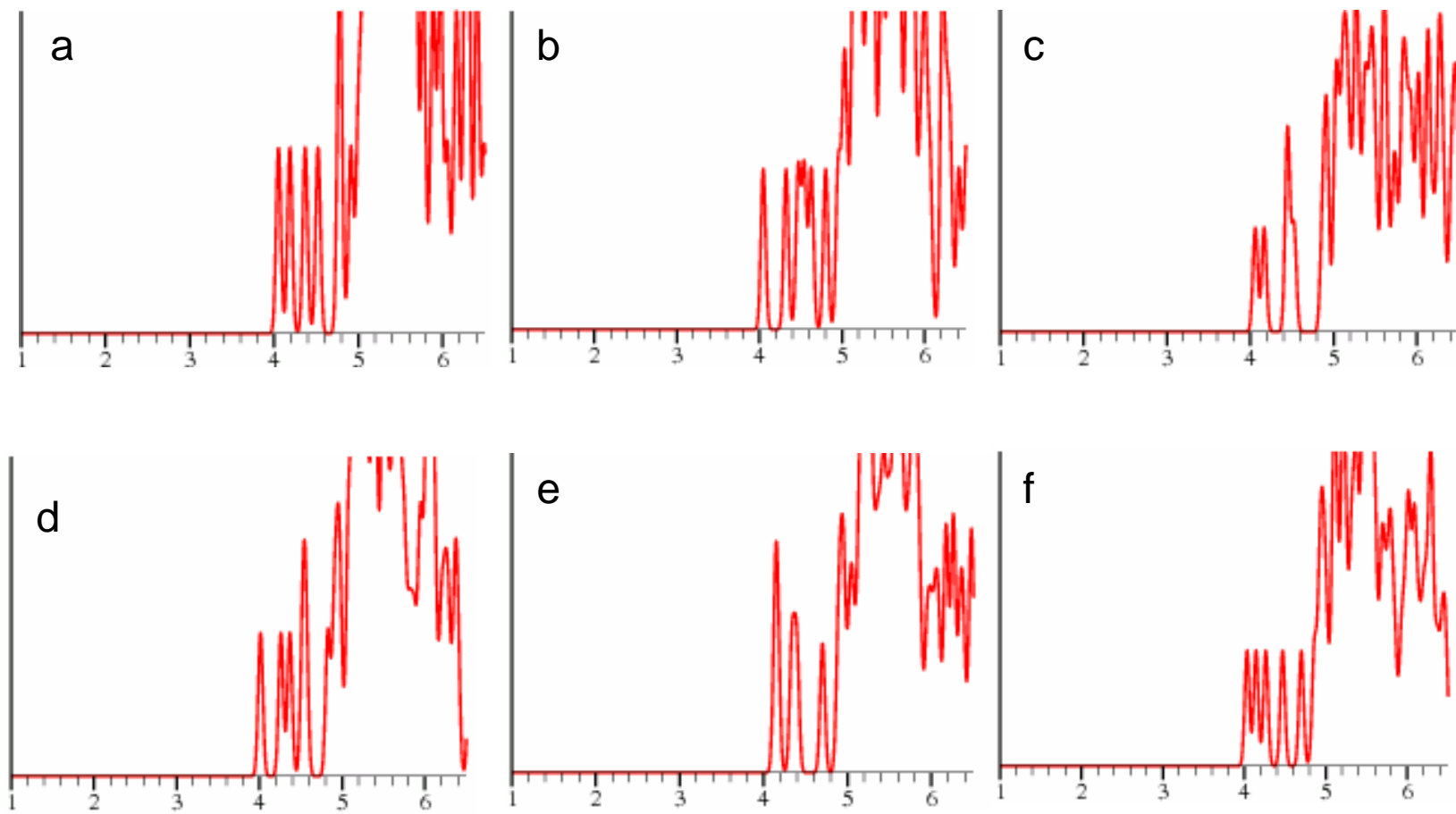
Au_{15}^- (top 5)

Figure 4A



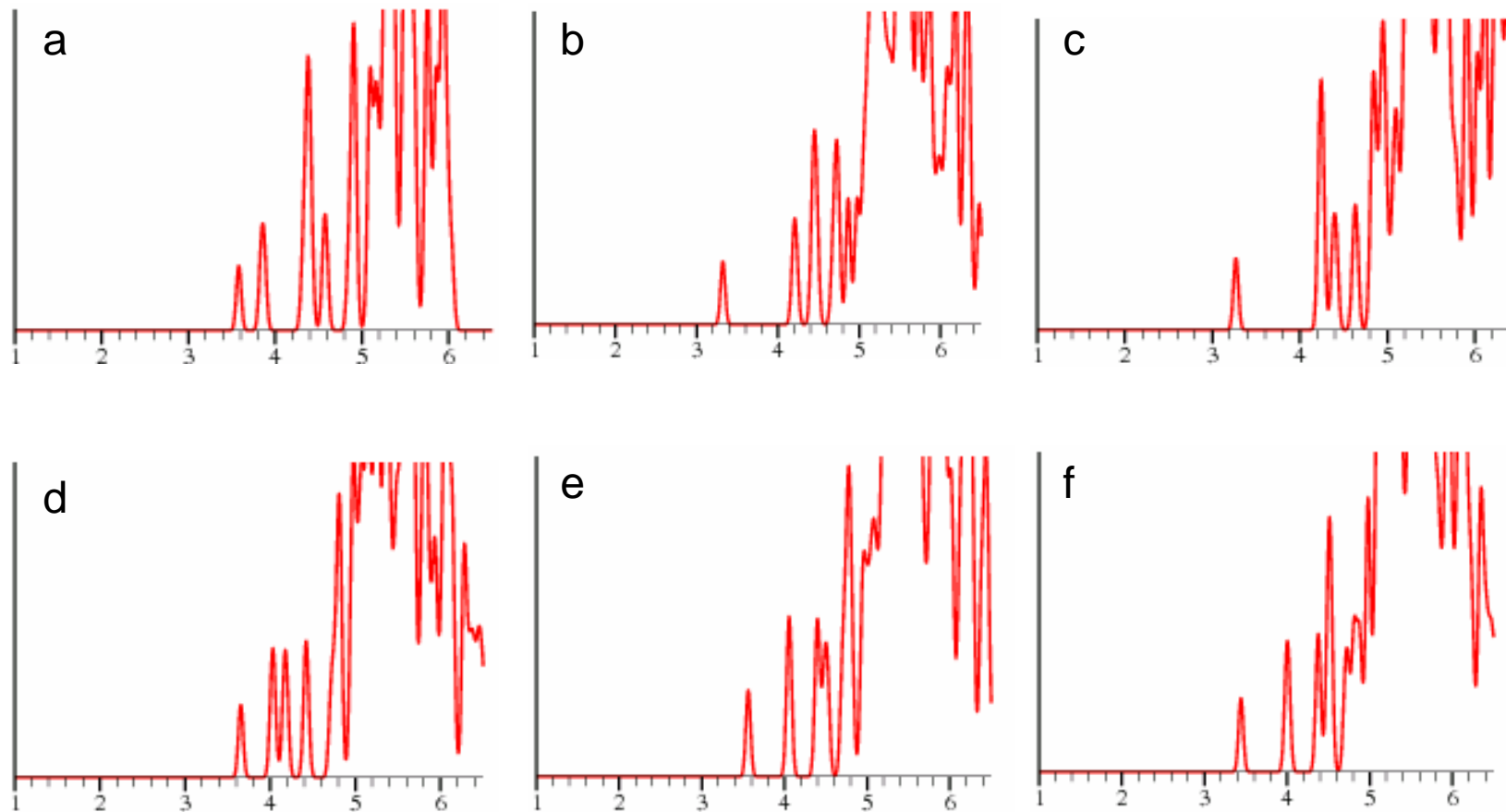
Au_{16}^- (top 5)

Figure 4B



Au_{17}^- (top 6)

Figure 4C



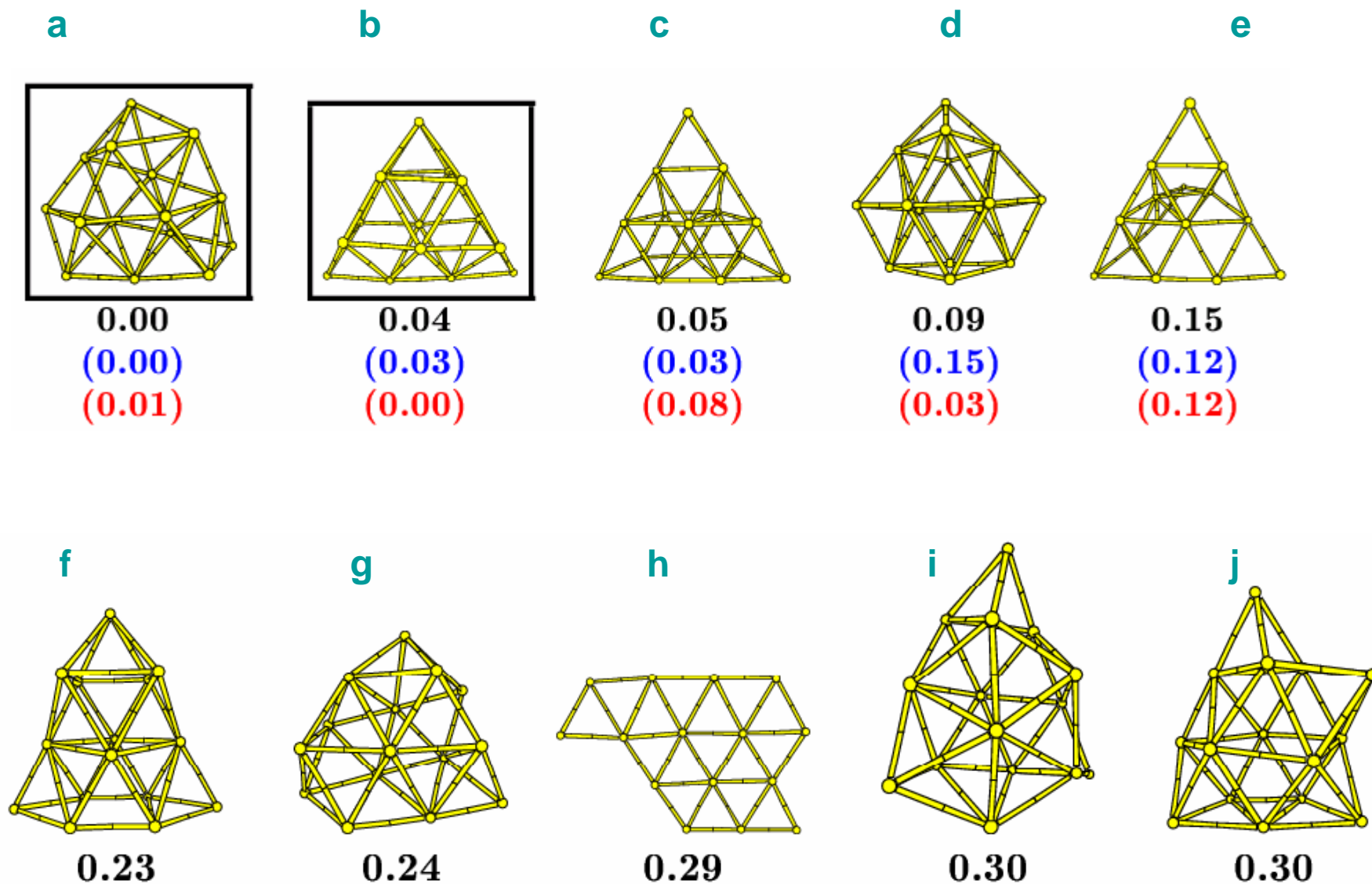
Au₁₈⁻ (top 6)

Figure 4D

Fig. 4. Top-10 lowest-energy isomers of Au₁₅⁻ (A), Au₁₆⁻ (B), Au₁₇⁻ (C), Au₁₈⁻ (D), and Au₁₉⁻ (E) obtained from a basin-hopping global search combined with DFT optimization and total-energy calculation. The energy values (in eV) given beneath each isomer are the relative energy with respect to the leading lowest-energy isomer. The energy values in black are based on the PBE exchange-correlation functional (1), and the double numerical basis set with polarization functions, implemented in the DMOL³ package (2). Those isomers with their energy value within 0.2 eV from the leading lowest-energy isomer are all regarded as candidates for the lowest-energy structure to be compared with experimental data. Relative energies among these candidate lowest-energy isomers are further evaluated by using a modest and a large basis sets. The energy values in blue are based on optimization with the PBEPBE/LANL2DZ functional/basis set, implemented in the GAUSSIAN 03 package (3), and the energy values in red are based on single-point calculations at the PBEPBE/SDD+Au(2f)//PBEPBE/LANL2DZ level of theory, implemented in the GAUSSIAN 03 package (3). Here "SDD+Au(2f)" denotes the Stuttgart/Dresden ECP valence basis (4, 5) augmented by two sets of *f* polarization functions (exponents = 1.425, 0.468). The isomers enclosed by a black frame also are highlighted in Fig. 1B.

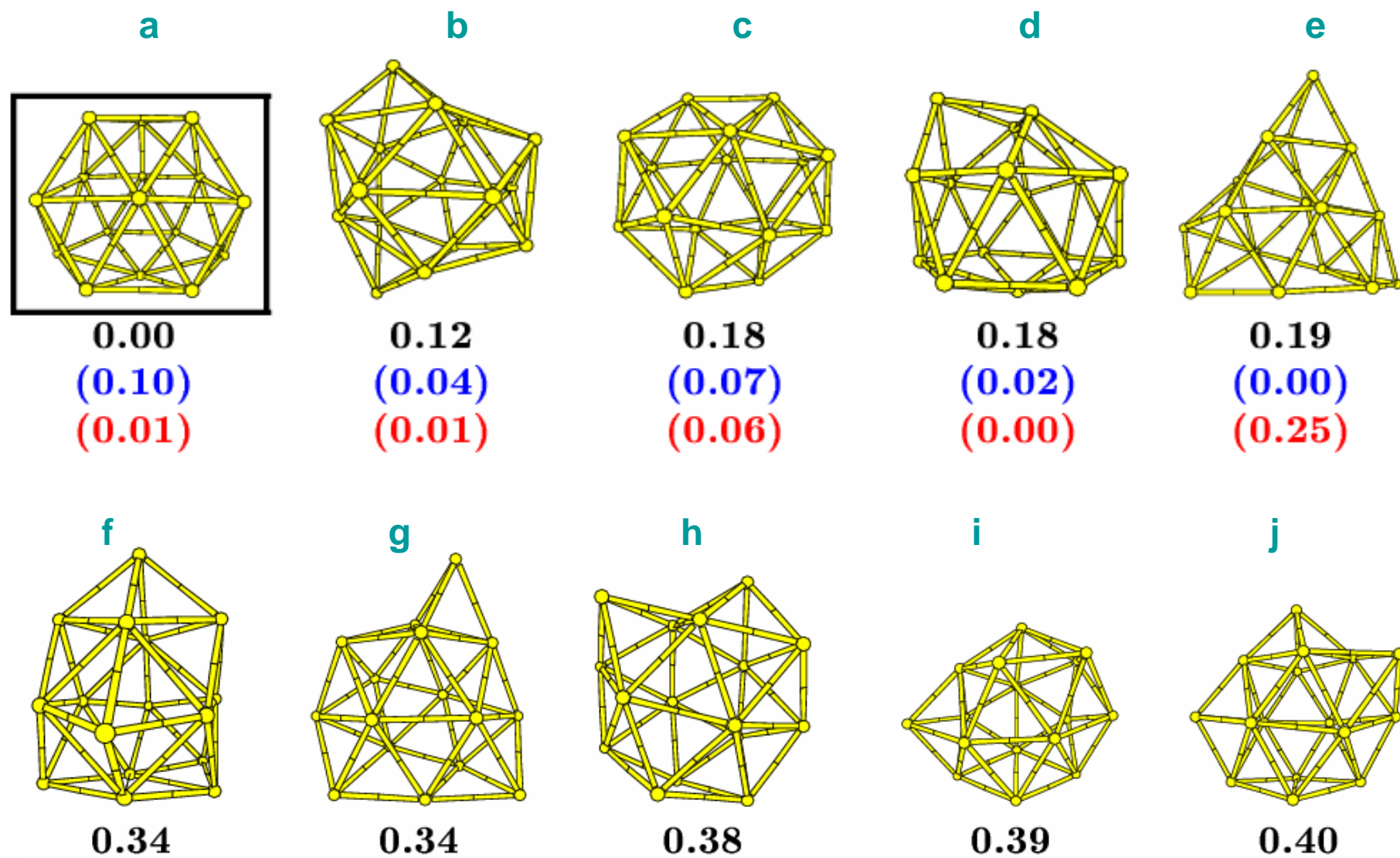
Notes

1. Perdew, J. P., Burke, K. & Ernzerhof, M. (1996) *Phys. Rev. Lett.* **77**, 3865–3868.
2. Delley, B. (1990) *J. Chem. Phys.* **92**, 508–517.
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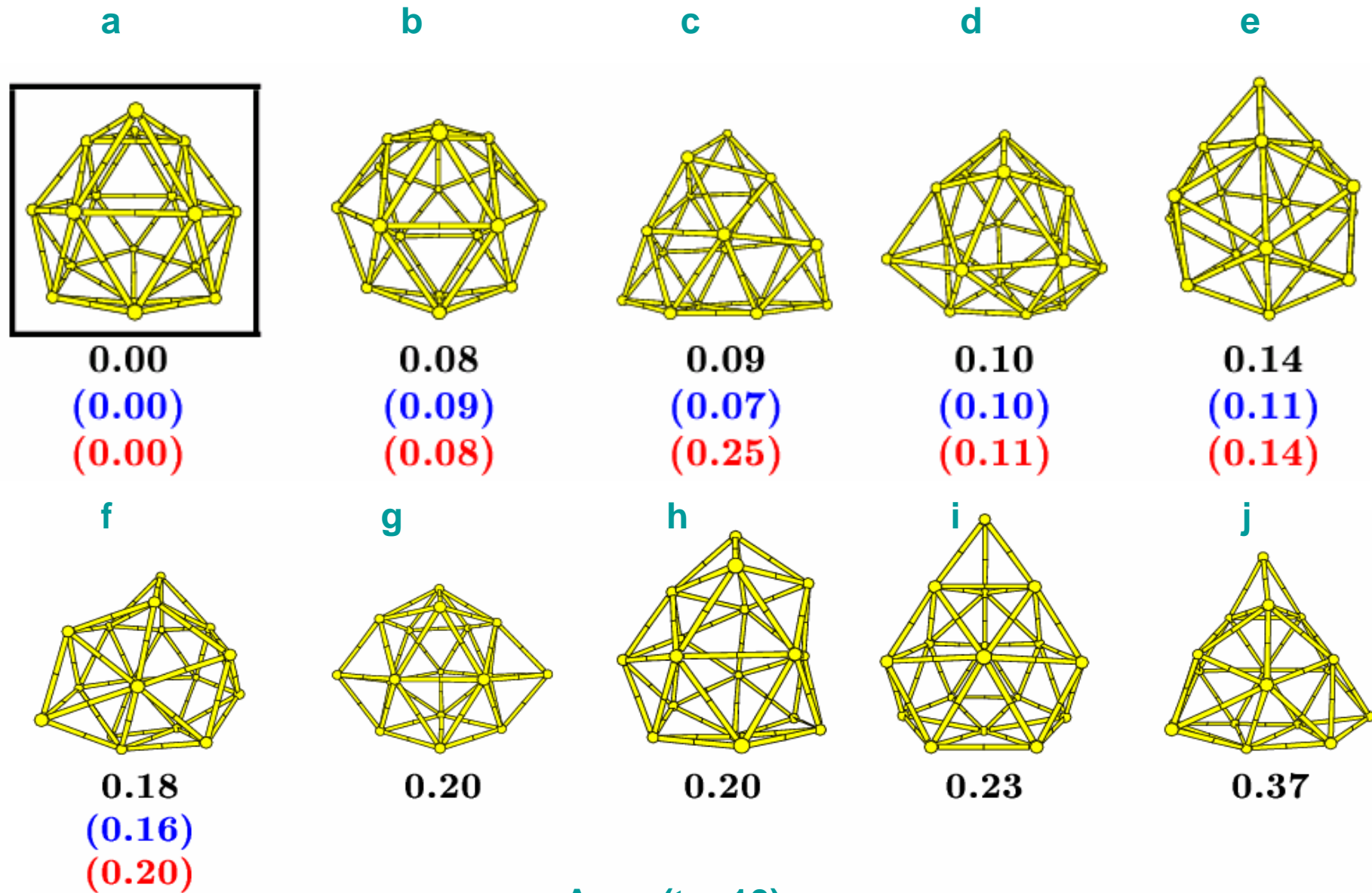
Au_{15}^- (top10)

Figure 3A



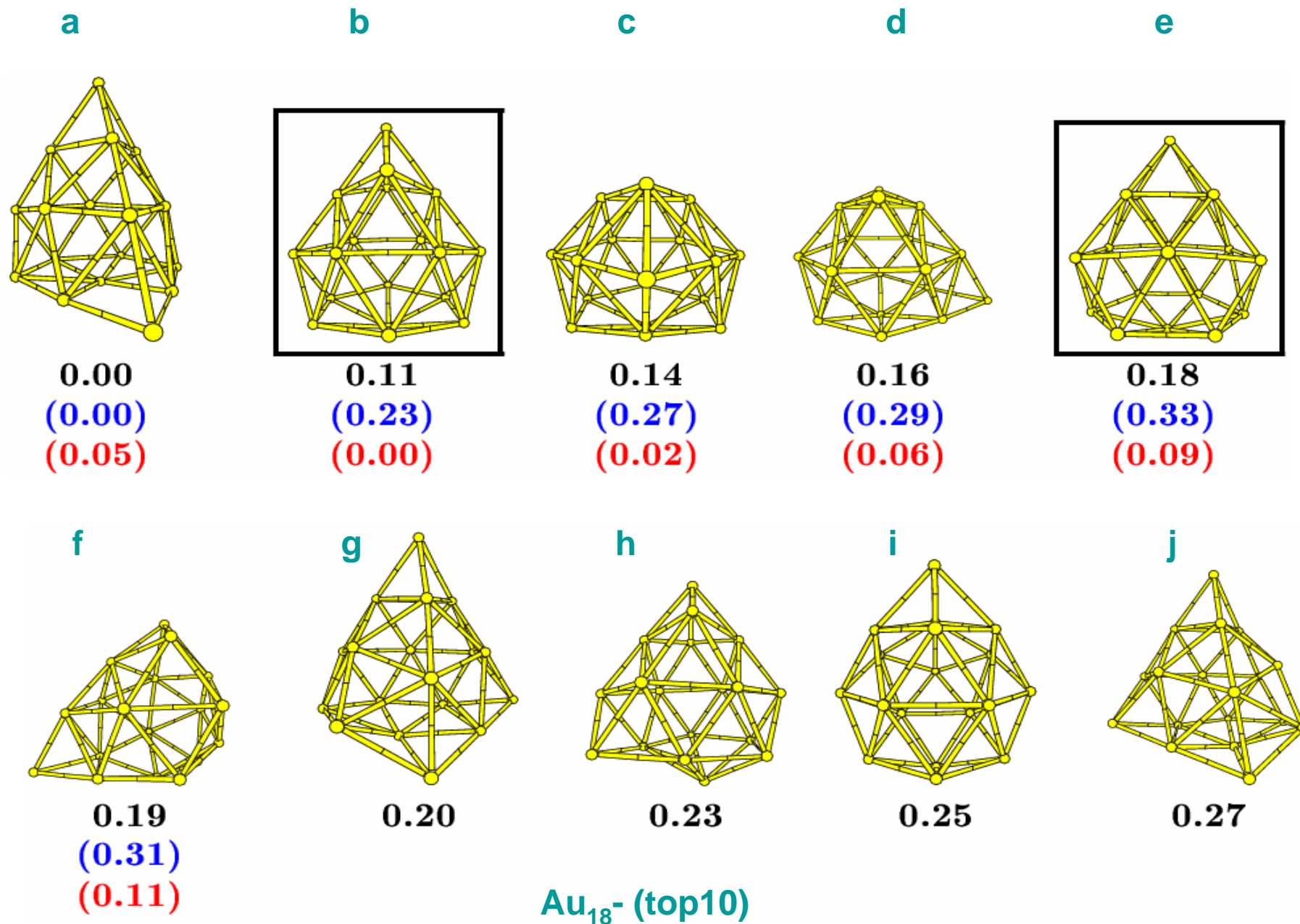
Au_{16}^- (top10)

Figure 3B



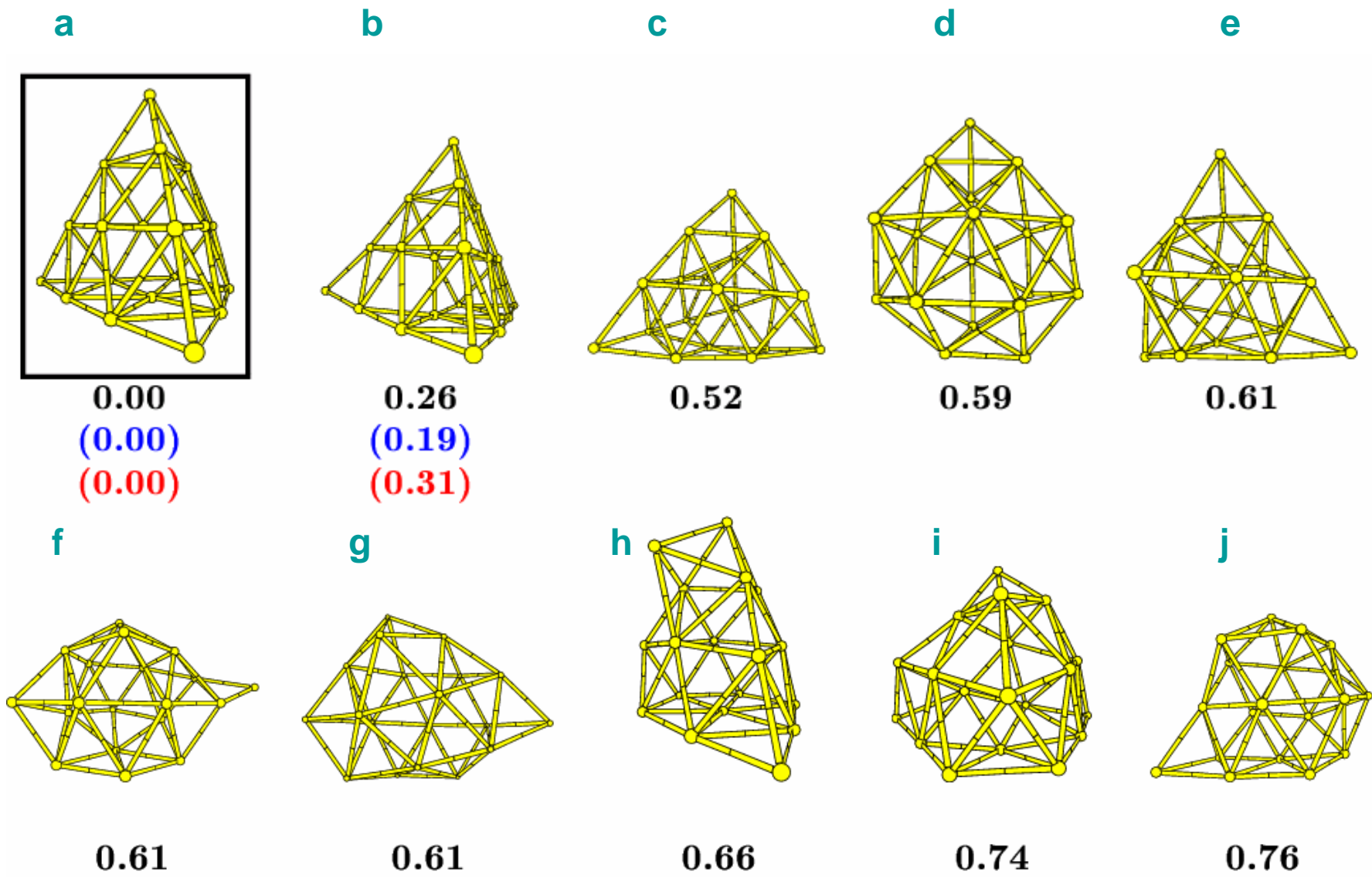
Au₁₇⁻ (top10)

Figure 3C



Au₁₈⁻ (top10)

Figure 3D



Au_{19}^- (top10)

Figure 3E

Table 2. The experimental adiabatic detachment energies (ADEs) for Au_n^- ($n = 15-19$) measured from the threshold of the first photoelectron band

Isomer	ADE, eV
Au_{15}^-	3.61 ± 0.03
Au_{16}^-	3.99 ± 0.03
Au_{17}^-	4.03 ± 0.03
Au_{18}^-	3.24 ± 0.03
Au_{19}^-	3.71 ± 0.03