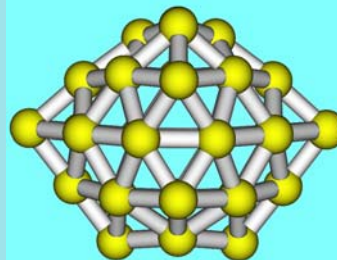


Au 34 Hollows

X. Gu^a, X. G. Gong^a,

^a Dept. of physics, Fudan University, Shanghai China, 200433

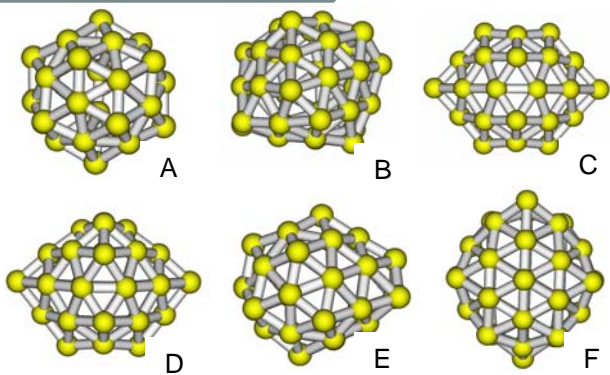


- Hollow cage
- Lowest energy
- Comparable Eg

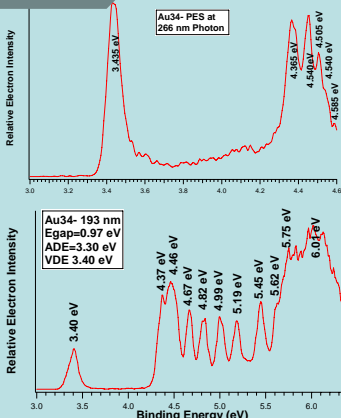
ABSTRACT

Gold hollow clusters are recently focused since a perfect Ih symmetrical cage cluster-Au32 is predicted¹. Although Au32 couldn't be found in the PES experiments due to the entropy effect cause of the temperature², Au34 may be the candidate that follow the experimental PES spectrum. A hollow cage-like gold-34 cluster, in our theoretical results, has the lowest binding energy and a very large energy gap, which is comparable to the experimental results.

STRUCTURES



PES



Egap = 0.97 ± 0.03 eV

ADE = 3.30 ± 0.03 eV

VDE = 3.40 ± 0.02 eV

ADE (Electron Affinity)

Expt. by Wang L.S. in
Dept. of physics,
Washington State University

RESULTS

Unit : eV

	A	B	C	D	E	F
E	-88.83	-88.33	-88.96	-89.07	-88.34	-88.47
Eg	1.53	0.17	0.74	0.98	0.15	0.56

One 'amorphous' structure: -88.58 (3 inner atoms)

METHODS & CONCLUSION

Theoretical calculation are based on the DFT with GGA implemented in the VASP code, with the PAW Pseudopotentials, and a scalar relativistic effect was included. A sc cell of 30 Å edge length with PBC, and the Gamma point approximation for Brillouin zone sampling and it's spin non-polarized

A cage structure of Gold cluster-34 is found to be the most stable structure, and has the comparable energy gap with the experimental PES. Once again, the relativistic effect of the heavy gold element is responsible to the stability of the cage structure. And it could be now believed that the Au34 is the first viewed metal-formed 'cage'.