Magic Number 32: A Shell Jellium Model Study

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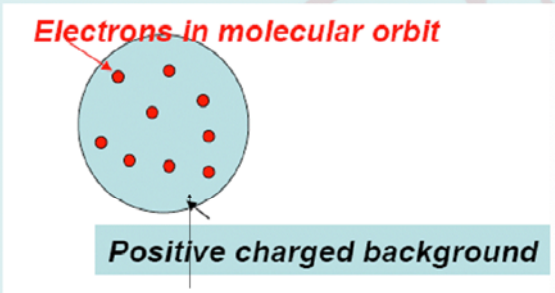
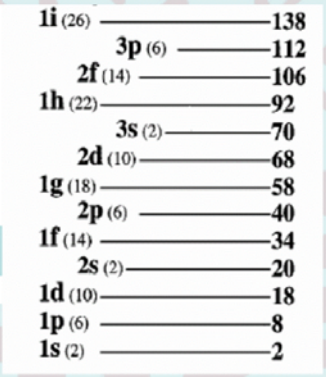
The spherical jellium model has been greatly successful in explaining experimental abundances of simple and noble metal clusters since the pioneering work of Knight on alkali-metal clusters. This model predict relatively large experimental abundance spectrum peaks when number of electrons is equal to 2, 8, 18, 20, 34, 40 and 58 etc, which are called "magic numbers". Recently, density functional theory predicted some stable cage-like cluster Au_{32}, Au_{42}, Au_{50}. These abnormal magic numbers are not found in the spherical model above. We construct and study shell jellium model, compare it with spherical one and show that jellium model can give proper explanation to these hollow structures with new magic numbers.

Jellium Model

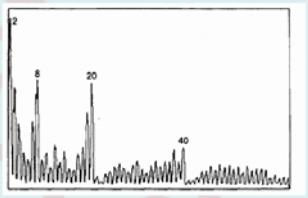


Specific ion structures are ignored and replaced by uniform positive background

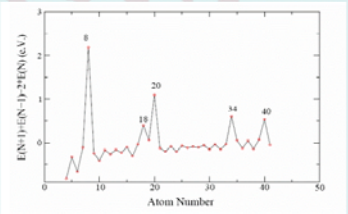
Electronic orbital sequence:



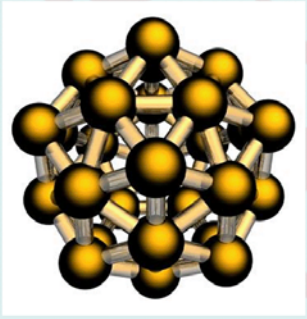
Experimental abundance spectrum of sodium clusters:



Corresponding spherical jellium model prediction:

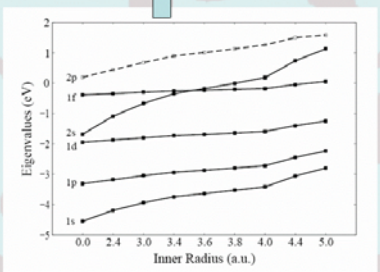


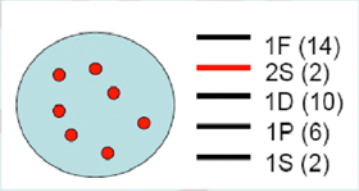
The cage-like structures of Au_{32} clusters predicted by recent density functional calculation:

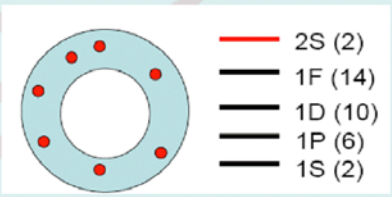


- The same group symmetry with C60
- Large HOMO-LUMO gap as 1.5 eV
- Large energy advantage to other isomers

Why is the cage stable?







Conclusion: Using the methods of density functional theory and shell jellium model, we show that energy levels of cluster s-electrons will rise with the existence of hollow cage, which might change certain electronic shell closure number. This model gives straightforward explanation for the stability of 32-electron systems and is verified by several of recent found golden cage-like structures and selected isomers of metal clusters with 32 valence electrons.

References:

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[2] W. D. Knight, K. Clemenger, W. A. de Heer, W. A. Saunder, M. Y.Chou, M. L. Cohen, Phys. Rev. Lett. 52, 2141 (1984)

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