Static and dynamical properties of Gold clusters using the Many-Body Alloy Hamiltonian

Luis Rincón
Departamento de Química, Facultad de Ciencias, Universidad de Los Andes, La Hechicera, Mérida-5101, Venezuela

The experimental and theoretical study of gold clusters is a subject of current interest.[1] Part of this interest arises from their use as a tip, or contact, in molecular circuits. Thus, it is well known that small clusters play a crucial role in experiment of molecular conductance. In these experiments, is assumed that the final contact is formed by only a small number of gold atoms. Beside this, there is also a more basic interest in the study of gold clusters. This is so, because, in most cases, the electronic properties and structures of small metallic clusters reveal little resemblance with their corresponding bulk properties and, at the same time, they show important difference with respect to those isolated atomic or molecular systems.[2] This, the study of metallic clusters opens some issues which are not met neither in molecular or solid state physics.

It is the main purpose of this work to explain some interesting periodic trends of Au clusters as a function of the cluster size using the many-body alloy Hamiltonian method of Zhong, Li and Tomanek.[3] This method is based in the second moment approximation to the band energy component of the cohesive energy, and is computationally very fast. The empirical parameters of the method were fitting in order to reproduce the fcc and bcc APW total-energy results for Au. The total energy of the method after the fitting procedure was less than 1 mRy than the APW one. The bulk modulus and equilibrium volume are in very nice agreement with APW calculation. With this parametrization we calculate, using Monte Carlo simulations, the cohesion energy, the magic numbers, stability of atomic structures as a function of the cluster size in the range from 1 to 10^6 atoms. In addition, we performed molecular dynamics simulation at various temperatures to obtain the dependence of the molecular properties with the temperature. We tested the transferability of the model by simulating the liquid Gold. Whenever possible we compared these results to experimental values.

References

1. N. Sierralta, L. Rincón and R. Almeida, "Energetic and Molecular Structural Properties of Small Gold Clusters", *Revista Mexicana de Física*, in press (2003).
2. L. Rincón, "Minimum-energy configurations of metallic clusters obtained by simulated annealing molecular dynamics using an Extended-Hückel Hamiltonian", *Revista Mexicana de Física*, **47**, 54 (2001).
3. D. Tomanek, S. Mukherjee and K. H. Bennemann, "Simple theory for the electronic and atomic structure of small clusters", *Phys. Rev. B28*, 665 (1983).