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Algorithm based on the Thomson problem for determination of equilibrium structures of metal nanoclusters

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Metal nanoclusters (MNCs) are considered particles of diameter of around 1 nm, ranging from 3–40 metal atoms, which are becoming a subject of increasing interest. Selective catalytic properties, synthesis of nanoparticles, synthesis of quantum dots, and synthesis of compounds for tomography imaging cancer are just a few examples of the many applications of these compounds. Determination of the structure of the MNCs is of special interest, not only because of the inherent dependency on the structure of their physical and chemical properties on the structure but also because of so many isomers due to the multivalent character of the metal atoms. Therefore, the determination of the equilibrium structures of MNCs is a challenging task for both theoreticians and experimentalist. Design of new materials, especially those based on nanoclusters, requires a strong support of the quantum chemistry. A new algorithm for determination of equilibrium structures suitable for metal nanoclusters is proposed. The algorithm performs a stochastic search of the minima associated with the nuclear potential energy function restricted to a sphere (similar to the Thomson problem), in order to guess configurations of the nuclear positions. Subsequently, the guessed configurations are further optimized, driven by the total energy function using the conventional gradient descendent method. This methodology is equivalent to using the valence shell electron pair repulsion model in guessing initial configurations in the traditional molecular quantum chemistry. The framework is illustrated in several clusters of increasing complexity: Cu_7, Cu_9, Cu11 as benchmark systems, and Cu_{38} and Ni_9 as novel systems. New equilibrium structures for Cu_9, Cu_{11}, Cu_{38}, and Ni_9 are reported.

Recent Publications:

1. E Arias, E Florez, and J F Pérez-Torres (2017) Algorithm based on the Thomson problem for determination of equilibrium structures of metal nanoclusters. J. Chem. Phys. 146:244107.
2. R Jin, C Zeng, M Zhou, and Y Chen (2016) Atomically precise colloidal metal nanoclusters and nanoparticles: fundamentals and opportunities. Chem. Rev. 116:10346–10413.
3. S Mitzinger, L Broeckaert, W Massa, F Weigend, and S Dehnen (2015) Understanding of multimetallic cluster growth. Nat. Commun. 7:10480.
4. F Ferraro, J F Pérez-Torres, and C Z Hadad (2015) Selective catalytic activation of acetylene by neutral gold cluster of experimentally known gas-phase geometry. J. Phys. Chem. C 119:7755–7764.
5. G Guan, S Liu, Y Cai, M Low, M S Bharathi, et al. (2014) Destabilization of gold clusters for controlled nanosysnthesis: From cluster to polyhedral. Adv. Matter 26:3427.

Biography

Jhon Fredy Pérez Torres received his BS in Chemistry from Universidad de Antioquia in 2004, and PhD in Theoretical Chemistry from the Universidad Autónoma de Madrid in 2012. He was awarded the Colombian Science Prize Alejandro Ángel Escobar in 2012. From 2012 to 2016 he was a Research Associate in the Freie Universität Berlin. He is presently a Professor in the Universidad Industrial de Santander, Bucaramanga, Colombia.

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