QUANTUM CHEMISTRY SCREENING OF THE PHYSICAL AND CHEMICAL PROPERTIES OF TRANSITION-METAL NANOCLUSTERS

PRINCIPAL INVESTIGATOR

JUAREZ LOPES FERREIRA DA SILVA
São Carlos Institute of Chemistry
University of São Paulo (USP)

CO-PRINCIPAL INVESTIGATORS

Eudes Eterno Fileti
Kaline Rabelo Coutinho

ABOUT THE PROJECT

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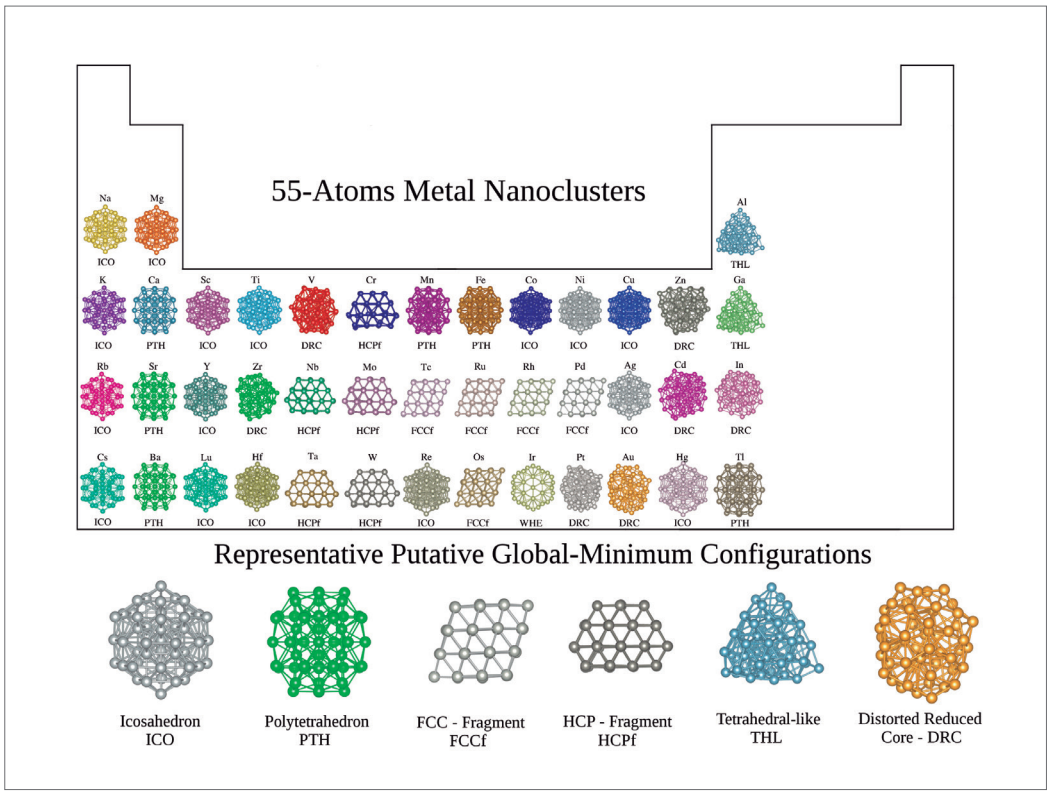
CONTACT

juarez_dasilva@iqsc.usp.br
http://qtnano.iqsc.usp.br

A large number of scientific achievements have been made in the field of nanoscience, and nowadays, it is possible to control the synthesis of transition-metal (TM) nanoclusters as a function of size (atom by atom), shape, and composition, charge state, etc. However, our atom-level understanding of the atomic structure, thermodynamic stability, electronic, and reactivity properties of TM nanoclusters as a function of size is far from satisfactory. In our group, Quantum Theory of Nanomaterials – QTNano, we have investigated the physical and chemical properties in gas-phase and under ambient conditions, e.g., temperature, of TM nanoclusters employing the state-of-the-art in quantum chemistry computational calculations. Beyond of those techniques, our group implemented from scratch the Revised Basin Hopping Monte Carlo (RBHMC), which have been employed to obtain putative global minimum configurations for nanoclusters, and the Parallel Tempering Monte Carlo, for temperature effects investigation.



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SUMMARY OF RESULTS

A large data base of nanoclusters configurations were build up by the RBHMC combined with empirical potencials for the TM systems, which was employed as candidate structures for density functional calculations. Based on that, we investigated the bebavior of the most important physical and chemical properties of TM clustes from n = 2 to 15 [1], and for 55-atom [2] nanoclusters. We identified the magic number clusters within the investigated size range, and found that 10 different structures can yield the putative global minimum configuration for 42 metal systems. Beyond of that, those systems were also the base for the study of nanoalloys, and we identified the compositions that leads to the high stability among several nanoalloys, e.g., PtFe, PtCo, PtNi, PtCu, PtZn [3], which is a key step to develop new nanocatalysts.

MAIN PUBLICATIONS

Chaves AS, Piotrowski MJ, Da Silva JLF. 2017. Evolution of the Structural, Energetic, and Electronic Properties of the 3d, 4d, and 5d Transition-Metal clusters (30 TM_n Systems for n= 2–15): A Density Functional Theory Investigation. *Phys. Chem. Chem. Phys.***19**: 15484-15502.

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Guedes-Sobrinho D, Nomiyama RK, Chaves AS, Piotrowski MJ, Da Silva JLF. 2015. Structure, Electronic, and Magnetic Properties of Binary Pt_nTM_(55–n) (TM = Fe, Co, Ni, Cu, Zn) Nanoclusters: A Density Functional Theory Investigation. *J. Phys. Chem.* **C 119 (27)**: 15669-15679.