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## IC28

## DFT investigation of the stability mechanisms of 8-atom binary clusters using machine learning

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Atomic clusters play a key role in nanoscience due to their unique properties that vary substantially with size, charge state, and composition. Particularly in the nanoscale regime, quantum-size effects can be promising for several applications in catalysis, such as methane dehydrogenation. (1) Those properties can be tuned by alloying two or more chemical species, nonetheless, there is a lack of efficient designing strategies from the theoretical area. In this study we propose a new methodology to understand the stability mechanisms of binary clusters using density functional theory calculations (DFT-PBE) and non-supervised machine learning. This methodology was employed to investigate AnB8-n binary clusters, where A, B = Fe, Co, Ni, Cu, Ga, Al, and n = 0, 2, 4, 6, and 8. To reach this goal, the generation of alloys was done from enumeration of homotops based on the unary clusters' geometries from previous studies (2) combined with a *k-means* clustering algorithm approach, enabling the performance of DFT calculations for only 2% of the possible homotops. (3) Moreover, from a Spearman Correlation analysis within our results were unveiled the properties that lead to the lowest energy configuration for each system, i.e., the stability mechanisms. Thus, this work contributes to the development of new functional materials and allows a similar procedure to be extended for other sizes and compositions.

**Palavras-chave:** Binary clusters. DFT-PBE. K-means clustering algorithm.

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