Nanoscale physics

The impurity effect at the cubic iron nanocluster growth

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The influence of impurity atoms into energy of cubic iron nanocluster upon adhesion of the iron atoms from the environment was studied by the method of molecular mechanics using Lennard-Jones potential [1]. We established that the energy of the system depends on the arrangement of impurity atoms according to associating of the iron atoms [2]. Was calculated most energetically favorable configuration of atoms, which correspond to increasing of the nanocluster on account of adhesion. The terms of the stability of the FCC and BCC nanoclusters as to the interstitial and substitutional impurities influence were estimated.

The study may be useful for nano-constructing clusters for use in medicine, biology and NEMS.

1. *Ramachandran K.I., Deepa G., Namboori K. Computational chemistry and molecular modelling: principles and applications. Springer: Heidelberg, 2008.*
2. *Husic B.E., Schebarchov D., Wales D.J.* Impurity effects on solid-solid transitions in atomic cluster // Nanoscale.-2016.-**8**.-P. 18326-18340.