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Stability of catalitic TM-nanoclusters $TM_{147-561}$:Ni,Pd (2D-spacers)

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Abstract

In this paper, using physically reasonable potentials, we conducted computer molecular dynamics simulation of heating the face-centered cubic lattice (FCC) of nanoclasters $TM_{147-561}$:Ni,Pd and detected specific thermal dimensional effects of structural stability loss initiated by isomeric transformation of FCC-cube octahedrons into icosahedrons.

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