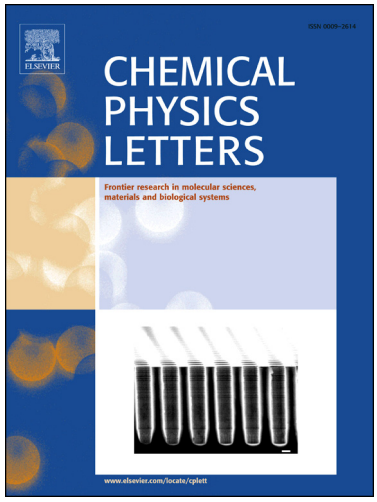

Frontiers article

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Conformation and catalytic activity of nickel–carbon cluster for ethanol dissociation in carbon nanotube synthesis: *ab initio* molecular dynamics simulation

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Abstract

Conformation and catalytic activity of nickel–carbon binary clusters are investigated to shed light on important questions on the carbon nanotube growth. Carbon atoms tend to stay at the surface of the binary cluster and form carbon chains with increasing carbon concentration. The binary clusters have lower catalytic activity for ethanol dehydrogenation compared to pure nickel clusters due to the strong electron negativity of carbon atoms. Moreover, the C–C bond dissociation in typical fragment molecules, which is a key reaction of carbon nanotube growth via alcohol CVD, is inhibited on the binary cluster due to the increase of the backward reaction.

Keywords

Ab initio molecular dynamics simulation; Carbon nanotube growth; Ethanol; Dehydrogenation; Nickel–carbon binary cluster

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