

Abstract Submitted
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Novel polyicosahedral Si nanowire: A molecular-dynamics study.

KENGO NISHIO, TETSUYA MORISHITA, WATARU SHINODA, MASUHIRO MIKAMI, Research Institute for Computational Sciences, National Institute of Advanced Industrial Science & Technology, Japan — A novel polyicosahedral nanowire, which is composed of linked icosahedral Si nanodots is spontaneously formed in a series of annealing molecular dynamics simulations of liquid Si inside a nanopore of 1.36 nm in diameter[1]. The polyicosahedral Si nanowire is stable even in a vacuum up to about 77% of the melting temperature of bulk Si. Our structural energy calculations reveal that the polyicosahedral nanowire is energetically advantageous over the pentagonal one for a wire whose diameter is less than 6.02 nm, though the latter has been recently proposed as the lowest energy wire. These results suggest the possibility of the formation of a new stable polyicosahedral Si nanowire.

[1] J. Chem. Phys. 125, 074712 (2006).

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