A Density Functional Theory Study of Selfassembled (InN)12n (n=1-9) Nanowires and Nanosheets: Implications for CO2 Capture and Optoelectronic Applications

RN Zhao[1], Rui Chen[1], Fan Lin[1], and Ju-Guang Han[2]

[1]Shanghai Dianji University
[2]University of Science and Technology of China

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Abstract

Geometries and electronic properties of selfassembled (InN)12n (n=1-9) nanosheets or nanowires are investigated at the PBE1PBE level. The growth patterns of semiconductor InN nanocrystal are revealed. Relative stabilities of (InN)12n (n=1-9) are studied. The even-numbered (InN)12n (n is even) nanoclusters have stronger stabilities than the neighboring odd-numbered (InN)12n ones. The particular stable geometries are assigned as the (InN)48 nanosheet for selfassembled film nanomaterials. The calculated energy gaps exhibit even-odd oscillation and reveal that (InN)12n (n=1-9) semiconductor nanoclusters are apparently good optoelectronic or energy nanomaterials; Furthermore, (InN)12n nanoclusters with energy gaps at the visible regions have potential applications in microelectronic and optoelectronic nanodevices. The slightly varied energy gaps for (InN)12n nanowires reveals they maintain individual (InN)12 properties. The calculated charge-transfers for (InN)12n (n=1-9) reflect that their ionic bonding enhances the stabilites of nanoclusters and that ionic bonding in (InN)12n (n=1-9) nanoclusters exists with covalent.

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