Structural properties of CdS nanocluster by using ab-initio molecular dynamics simulation.

Aim

We illustrate a calculation procedure to describe the geometrical and structural properties of CdS-Cd by means of ab initio molecular dynamics simulations, using standard Car-Parrinello scheme.

Direct semiconductor Large band gap Several applications in optoelectronic devices
Several electronic, structural and geometrical properties size-dependent
Three Crystallographic Form For Bulk CdS: hexagonal, cubic, rocksalt

Literature Data

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<td>rocksalt</td>
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<td>3.0-4.0</td>
<td>3.0(RO)-7.0(TEM)</td>
<td>4.2</td>
<td>~1.3</td>
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CdS Wurtzite Bulk

1) Setting

-pseudopotentials, box size,

-exchange-correlation functional,

-wave plane cutoff


3) Determination of the crystallographic and energetic parameters for bulk structure

4) Build, of CdS cluster 96 atoms, 48 Cd and 48 S, performing molecular dynamics from 100K to 600K

Size around 2.0 nm

Results

-A novel computational approach to study nanostructured CdS semiconductor by means of ab initio molecular dynamics has been presented.

-Pseudopotential, exchange-correlation functional, cutoff and box size were chosen in order to achieve satisfactory agreement with experimental results on CdS cluster and dimer.

-Small CdS clusters were built by the authors with 96 atoms, with around 2.0 nm in size. A calculation system was found, including the conjugate gradient method, at 1000 K and 600 K.

-Wave function distributions and coordination numbers were obtained that enabled the structural properties of CdS atomic species to be calculated.

-Surface structural modifications of CdS nanoclusters have been investigated, using standard Car-Parrinello molecular dynamics simulations.

References


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