

Synthesis of Inorganic Structural Isomers by Diffusion-Constrained Self-Assembly of Designed Precursors: A Novel Type of Isomerism

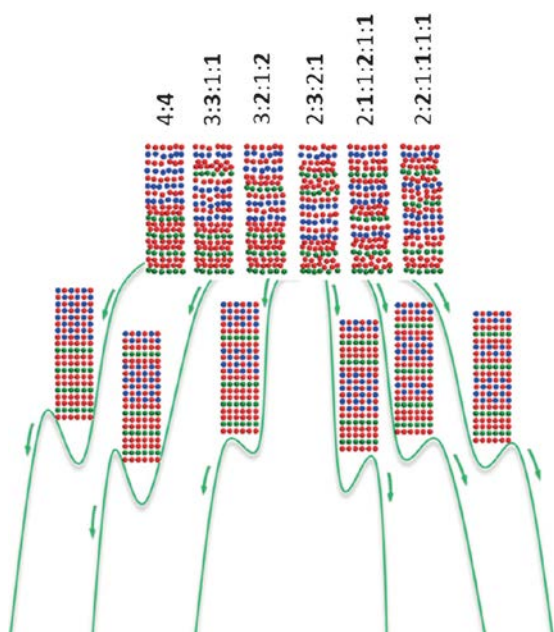
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Hot paper

Short Abstract

The structure of precursors is used to control the formation of six possible structural isomers that contain four structural units of PbSe and four structural units of NbSe₂. The electrical properties of these compounds vary with the nanoarchitecture. For each pair of constituents, over 20 000 new compounds, each with a specific nanoarchitecture, are possible with the number of structural units equal to 10 or less. This provides opportunities to systematically correlate structure with properties and hence optimise performance.



Above. Schematic representation of the free-energy landscape for the formation of the six isomers of $[(\text{PbSe})_{1.14}]_4(\text{NbSe}_2)_4$. The images at the top depict the structures of the initial reactants. The images in the middle depict idealised atomic structures of the six isomers formed on annealing. The green lines show the energy pathways for the six different reactants transforming into the six different targeted compounds.