Computational Exploration of Polymorphism in Tetrahedrally Coordinated Semiconductors

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Tetrahedrally coordinated semiconductors provide numerous textbook examples of polymorphism. The low pressure polymorphs of ZnS, zincblende and wurtzite, provide the common names for the B3 and B4 structure types, while at high pressure many of these materials adopt stable six-coordinate (rocksalt, B1) or even eight-coordinate (CsCl, B2) polymorphs.

A long standing question is whether this experimentally known polymorphism describes the full set of accessible structures, or whether more exotic structures may exist? And if so, what synthetic conditions might be used to access (meta-)stable materials?

Computational modelling offers a powerful tool for exploring both these questions, and a rich theoretical polymorphism has been revealed to exist for many tetrahedral semiconductors (e.g. [1–3]).

In this talk, I will discuss three areas of my own work in this area, including:

• The effect of reducing crystal dimensions to the nanoscale domain, and how this affects the stability of competing polymorphs in thin film ZnO [4].

• Computational exploration of epitaxial growth strategies for templating metastable exotic polymorphs in ZnO, ZnS, and CdS thin films [5].

• Enumeration of “bond-alternation” motifs as a systematic approach to explore bulk polymorphism of ZnO [6].

Bibliography

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