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Phase stability of ZnO from first-principles calculations

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Abstract
First-principles calculations of the phonon dispersion relations and the phonon density of states for ZnO polymorphs: wurtzite, zinc-blende, rocksalt structures, and as yet the experimentally undiscovered CsCl structure, are presented. All the phases were exposed to pressures ranging from 0 to 20 GPa. The pressure–temperature phase diagram of ZnO was constructed and compared to experimental data, where available.

