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Quantum Monte Carlo (QMC) study of Pressure-induced B3-B1 phase transition in GaAs

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Abstract content
 (Max 300 words)

We have investigated the transition pressure, p_t , of bulk GaAs from the zinc blende (B3) to the rocksalt (B1) structure using the local density approximation (LDA), generalized gradient approximation (PBE-GGA) and diffusion Monte Carlo (DMC). We took into account finite temperature effects (zero-point vibrational effects) as well as finite size corrections. DMC projection starting from GGA trial nodal surface supports the higher value of the transition pressure (~ 17 GPa) than the lower value of (~ 12 GPa), both of which are experimentally reported values. This projection increases the transition pressure, p_t , from DFT predictions, being of the same tendency as that for Si bulk crystal. The choice of the XC functional in DFT was found to significantly determine the phase transition pressure, DMC gave more accurate results for this transition pressure.

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PhD

Main supervisor (name and email)
and his / her institution

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No

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