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B3-B1 phase transition in GaAs: A Quantum Monte Carlo Study

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The pressure induced B3-B1 phase transition has been studied using both density functional theory (DFT) and quantum Monte Carlo (QMC) methods. We present results obtained using the local density approximation (LDA), PW91-GGA generalized gradient approximation, hybrid density functionals and QMC. The changes in the equation of state has also been investigated using the different functionals and from the results obtained, we find that the choice of functional significantly effect the to the equation of state. The results of the B3-B1 phase transition pressure for DFT using the different functionals and QMC are reported and they demonstrate good agreement with experimental data.

**Level (Hons, MSc,
 PhD, other)?**

PhD

**Consider for a student
 award (Yes / No)?**

Yes

**Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?**

Yes

Primary author: Mr OUMA, Cecil (Student)

Co-authors: Dr AMOLO, George (Computational Materials Sciences Group, Department of Physics, Moi University,); Dr MAPELU, Joseph (Computational Materials Sciences Group, Department of Physics, Moi University,); Dr MAKAU, Nicholas (Computational Materials Sciences Group, Department of Physics, Moi University,); Dr MAE-ZONO, Ryo (School of Information Science, Japan Advanced Institute of Science and Technology, Asahidai 1-1, Nomi, Ishikawa 923-1292, Japan)

Presenter: Mr OUMA, Cecil (Student)

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