Contribution ID: **82** Type: **Oral**

The structural phase transition of Ga(Mn)N under high pressure

Thursday 25 May 2017 08:55 (15 minutes)

Gallium nitride doped with small concentration of manganese (Ga_xMn_{1-x}N) is one of the most diluted magnetic semiconductors which used for the spintronic applications. In this work, the Ga₃₁Mn₁N₃₂ in the zinc-blende (ZB) and rocksalt (RS) structures were investigated. We employed the *ab*-initio density functional theory (DFT) within the generalized gradient approximation (GGA) to study electronic and magnetic properties, such as the band structure, the density of state and the magnetic moment. The structural phase transitions under pressure up to 60 GPa were also studied. We found that the Ga₃₁Mn₁N₃₂ in ZB phase is stable at ambient pressure, and change to the RS phase about 42 GPa. Finally, our calculations are in consistent with other experimental and theoretical literature.

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Session Classification: A6: Condensed Matter and Accelerators

Track Classification: Condensed Matter Physics