Magnetic Properties of (Cr,Ga)N Diluted Magnetic Semiconductor

J. RUFINUS, Widener University, Chester, PA 19013 — We study the magnetic properties of Cr-doped GaN Diluted Magnetic Semiconductor (DMS) using first principles Density Functional Theory. The effect of Cr clustering on the magnetic properties of this DMS material was investigated. We found that the Cr atoms tend to bind more strongly to N atoms than to Ga atoms, resulting in larger overall magnetic moments and lower total energy. This may explain the role of the anions in this DMS material.

1Work supported in part by NSF (Grant No. ECS-0609129) and Pittsburgh Supercomputing Center (Computational Grant No. DMR-050028P)