Abstract of Presentation

Presentation Title:

Cation Vacancies in Nitride Semiconductors: A Possibility of Intrinsic Ferromagnetism

<u>Abstract</u>:

Nitride semiconductors such as GaN and InN have emerged as new materials for blue light-emitting and laser diodes and now prevailed as most important semiconductors in optoelectronics. Recently, ferromagnetic behaviors at well above room temperature have been also reported for magnetic-impurity doped GaN, offering a new stage for interactions among charge, spin, and light. The magnetic behavior in the material is quite different in quality from the previous II-VI and III-V magnetic semiconductors so that the clarification of the microscopic origins for the ferromagnetic state in GaN is important.

In this talk, I report the density-functional-theory based electronic-structure calculations for atomic vacancies in Gd-doped GaN and also in Gd-free GaN, AlN and InN. We have found that the cation vacancy in these materials exhibits spontaneous spin polarization. We have further examined a variety of spin and geometrical configurations for Ga vacancies in GaN, and found that the Ga vacancies interact with each other ferromagnetically and that the magnetic moment increases linearly with increasing the number of Ga vacancies. The results indicate an unprecedented magnetism due to atom vacancies in covalent semiconductors.