Materials Science and Technology Division

Materials Theory Seminar

"Theory of defects in photovoltaic materials"

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11:00 a.m.
Bldg. 3025M, Third Floor Conference Room

Abstract:
Defects in photovoltaic materials can strongly impact the efficiency of solar energy conversion. Understanding the formation mechanisms and resulting properties of these defects is important for improving solar cell performance. These defects also provide generic models for the formation mechanisms and properties of defects in other semiconductors. In this talk I will discuss my recent results for defects in two widely used solar cell materials, Si and GaAsN. I first discuss BO2 complexes in B-doped Si [1]. These complexes are nonradiative carrier-recombination centers, and are detrimental to Si solar cell efficiency. They are formed by light-induced O2 diffusion at room temperature. I show that recombination at BO2 complexes and the diffusion of O2 are both driven by self-trapping of electron and hole carriers. I next discuss the formation of a metastable hydrogen configuration in GaAsN which results from hydrogen irradiation or implantation [2]. Ion implantation is usually considered simply as an alternative way to boost the concentration of certain impurities. However, I will show that different impurity configurations may result from different methods for introducing impurities into a semiconductor. In GaAsN under H irradiation, the injected protons cannot quickly equilibrate with the electron reservoir even though the GaAsN sample is grounded. As a result, an injected proton will relax to the ground-state proton configuration whose conversion, upon subsequent charge neutralization, to the ground-state neutral H configuration is blocked by an energy barrier. Finally, I will discuss the formation of metastable N clusters in GaAsN [3], which are efficient exciton recombination centers. In particular, I will address the formation of these metastable N clusters, which may be mediated by hydrogen in the growth environment.

[1] M. -H. Du, H. M. Branz, R. S. Crandall, and S. B. Zhang, Phys. Rev. Lett. 97, 256602 (2006)
[2] M. -H. Du, S. Limpijumnong, and S. B. Zhang, Phys. Rev. B 72, 073202 (2005)
[3] M. -H. Du, S. Limpijumnong, and S. B. Zhang, Phys. Rev. Lett. 97, 075503 (2006)

Host: David Singh