KYOTO UNIVERSITY
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INTEGRATED
MATERIALS SCIENCE

グローバルＣＯＥ講演会

日時：　2010年6月28日（月）14:00～15:30

場所：　工学部物理系校舎 830セミナー室
（吉田キャンパス）

Overcoming the Doping Asymmetry Problem in Wide Gap Semiconductors

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Application of semiconductors as electric and optoelectronic devices depends critically on their dopability. Failure to dope a material, i.e., to produce enough free charge carriers beyond a certain limit at working temperature, is often the single most important bottleneck for advancing semiconductor-based high technology. Unfortunately, most wide-band-gap (WBG) materials such as ZnO or diamond experience the doping asymmetry problem, i.e., it can be either easily doped *n*-type or *p*-type, but not both. This asymmetry-doping problem has severely hindered the potential applications of these WBG materials. In this talk, taking ZnO as an example, I will discuss the origin of the p-type doping difficulty in ZnO and approaches to overcome the p-type doping difficulties in ZnO. These include (1) how to increase the dopant solubility, (2) how to design shallow p-type dopants and (3) how to modify the host band structures to reduce intrinsic defect-compensation. I will also discuss the techniques that have been used in our defect calculations to improve the cell size convergence, such as the mixed k-point scheme. The issue of band gap error and the approaches used to correct the band gap error will also be discussed.

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