Materials Science and Technology Division

"Optimal Dopant Control in Oxide Semiconductors for Spintronic and Solar Energy Applications"

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11:00 a.m.
HTML/4515, Room 265

ABSTRACT

In this talk, a combined computational and experimental approach will be presented to optimally control dopant in oxide semiconductors for spintronic and solar energy applications. First, we propose a new dilute magnetic semiconductor (DMS), carbon-doped ZnO. A magnetic moment of 2.02 μ_B/C, when carbon substitutes oxygen in ZnO, and ferromagnetic coupling among magnetic moments of the carbon dopants were predicted by first-principles calculations. The C-doped ZnO was experimentally confirmed to be ferromagnetic at room temperature by magnetic hysteresis loop and Hall Effect. Our first-principle calculations also predicted that C-doping could result in ferromagnetism of CdS. Secondly, a conceptually novel approach, termed non-compensated codoping, will be proposed to controllably narrow the band gap of TiO_2 for greatly enhanced photocatalytic activity in the visible light region. The concept is first demonstrated using first-principles calculations within density functional theory, and followed by compelling experimental evidences for its validity, as represented by direct scanning tunneling spectroscopy measurements of bandgap narrowing, dramatically enhanced optical absorbance, and photoactivity manifested by efficient hole-electron separation in the visible spectral region. We further investigate the bandgap engineering of GaN by the codoping method. Finally, the origin of phase-dependent photocatalytic activity of TiO_2 will be discussed based on the combined approach.

Host: Zhenyu Zhang (576-5346)

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