Physics Seminar

Michigan Technological University

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2:30 pm, Room G06 Rekhi Hall

Optimal Dopant Control in Compound Semiconductors for Spintronic and Energy Applications

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Abstract: Doping is very important for the application of materials in various fields. In this presentation, a conceptually novel approach, termed non-compensated codoping, will be proposed to control the dopant to be substitutional and engineer the bandgap. The concept embodies two central ingredients: The electrostatic attraction within the co-dopant pair enhances the thermodynamic and kinetic solubility in substitutional doping, and the non-compensated nature ensures the creation of intermediate electronic bands within the wide bandgap, effectively narrowing its value. Two examples will be presented. The first example is the design of photocatalyst for water splitting. We found that the codoping can controllably narrow the bandgap of TiO_2 for greatly enhanced photocatalytic activity in the visible light region. The design 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. The second example is the first-principles study on the magnetic property of codoped SiC for spintronics. We found that the codoped SiC can be either ferromagnetic or antiferromagnetic by controlling the codoping configurations. Nitrogen-TM (TM=Cr, Mn, Fe, and Co) codoping leads to ferromagnetism with a high exchange energy, while oxygen-TM codoped SiC is antiferromagnetic or non-magnetic, regardless that TM-doped SiC is ferromagnetic, antiferromagnetic, or non-magnetic. The ferromagnetism is attributed to the electron-mediated interactions because of the coupling between the spin-polarized TM-*d* and N-*p* electrons and the formation of the impurity band within the bandgap.

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