

Dual Nature Acceptors in Semiconductors: Small Polarons vs Shallow States in Gallium Nitride

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Abstract

Currently, only one shallow acceptor (Mg) has been discovered in GaN. Here, using photoluminescence (PL) measurements combined with hybrid density functional theory, we demonstrate that a shallow state also exists for the BeGa acceptor. A PL band with a maximum at 3.38 eV reveals a shallow Be-related acceptor level at 113 meV above the valence band, which is the lowest value among any dopants in GaN reported to date. Calculations suggest that the BeGa is a dual-nature acceptor with a shallow state and a strongly localized small polaronic state with a significantly lower hole capture efficiency. Using theoretical calculations in comparison with experimental PL measurements, we find several dual-nature acceptors in GaN. The physics of defects in semiconductors, theoretical approaches, experimental techniques, and the search for p-type wide bandgap nitrides are discussed in this talk.