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**Modeling Shallow Core-Level Transitions in the Reflectance Spectra of Gallium-Containing Semiconductors** NICHOLAS STOUTE, DAVID ASPNES, North Carolina State University, DE ASPNES GROUP TEAM — The electronic structure of covalent materials is typically approached by band theory. However, shallow core level transitions may be better modeled by an atomic-scale approach. We investigate shallow d-core level reflectance spectra in terms of a local atomic-multiplet theory, a novel application of a theory typically used for higher-energy transitions on more ionic type material systems. We examine specifically structure in reflectance spectra of GaP, GaAs, GaSb, GaSe, and $GaAs_{1-x}P_x$ due to transitions that originate from Ga3d core levels and occur in the 20 to 25 eV range. We model these spectra as a $Ga^{+3}$ closed-shell ion whose transitions are influenced by perturbations on 3d hole-4p electron final states. These are specifically spin-orbit effects on the hole and electron, and a crystal-field effect on the hole, attributed to surrounding bond charges and positive ligand anions. Empirical radial-strength parameters were obtained by least-squares fitting. General trends with respect to anion electronegativity are consistent with expectations. In addition to the spin-orbit interaction, crystal-field effects play a significant role in breaking the degeneracy of the d levels, and consequently are necessary to understand shallow 3d core level spectra.

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