Project Summary/Abstract

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Controlling recombination in wide-bandgap materials

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It has recently become clear that our current understanding of recombination processes at localized defects or impurities in solids is incomplete. Such recombination events govern loss mechanisms and reliability of devices and the quantum efficiency of light emitters, including single-photon sources for quantum information science. Work by the PI has revealed that excited states play a decisive role in nonradiative recombination, and hitherto neglected "impurity Auger" processes have a large impact. The proposed project is aimed at rigorously calculating the rate of these processes; using the acquired knowledge to significantly improve device performance; and validating the approach through experimental collaborations.

Correct inclusion of these mechanisms is particularly important in wide-bandgap materials, where current recombination models greatly underestimate the rates. Building on the PI's expertise, first-principles approaches for accurately calculating transition rates involving excited states and Auger processes will be developed. A fundamental understanding of these mechanisms is essential to suppress nonradiative recombination in wide-bandgap light emitters and power electronics. The methodologies will also support the characterization and design of efficient centers for applications in which radiative recombination underlies the functionality; these include phosphors, scintillators, and single-photon emitters for quantum information science.

Computational approaches will include density functional theory, hybrid functionals, the random phase approximation, and many-body perturbation theory. Experimental validation will be enabled through funded and unfunded collaborations. Nitride semiconductors will constitute the main materials platform used to construct and validate the approach, but applications are much broader. The ability to predict radiative and nonradiative rates will provide a framework for analyzing and controlling loss mechanisms in devices and emission processes in single-photon emitters. The proposed basic research on a transformative science issue will open new ways of thinking about recombination phenomena and lay a foundation for future new capabilities for DoD.