# Unveiling the Microscopic Mechanism of Mg Co-doped GAGG:Ce Scintillators: From Defect Thermodynamics to Quantum Optical Acceleration

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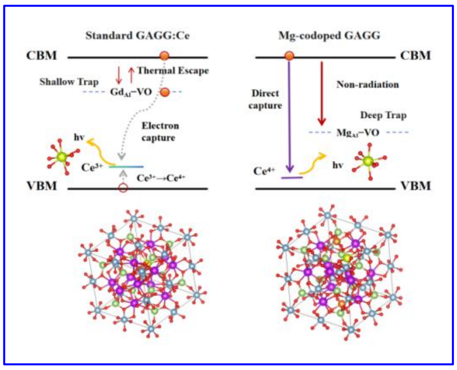
Mg co-doping is an effective strategy to improve the timing response of Ce-doped garnet scintillators; however, the microscopic origins of the associated light yield reduction and the precise acceleration mechanism at the atomic scale remain debated. In this study, we present a systematic investigation combining VASP first-principles calculations[1-2], thermodynamic modeling, and Geant4 Monte Carlo simulations[3].

Electronic structure calculations indicate that the complex formed by the antisite defect $Gd_{Al}$ and an oxygen vacancy ($Gd_{Al}$−VO) introduces localized shallow electron traps below the conduction band minimum, identified as the primary cause of delayed carrier recombination. Thermodynamic analysis confirms that Mg occupies Al sites with an overwhelming preference over Gd (by 11 orders of magnitude at the melting point) and exhibits strong repulsion towards oxygen vacancies. This thermodynamically suppresses the formation of $Gd_{Al}$ defects and their associated trap complexes, thereby mitigating the slow decay components. Crucially, optical property calculations reveal the quantum origin of the fast component acceleration: Mg-induced local lattice distortion (evidenced by Ce-O bond contraction) and the modified dielectric environment synergistically increase both the oscillator strength and refractive index for the Ce 5d→4f transition. This leads to a theoretical reduction in the intrinsic radiative lifetime by approximately 15%, which quantitatively aligns with experimentally reported fast decay values[4]. Furthermore, calculations reveal that Mg-stabilized $Ce^{4+}$ centers introduce charge transfer transitions that enhance parasitic absorption of the emitted light, explaining the reduction in light yield. Finally, Geant4 simulations, parameterized with these microscopic findings, demonstrate an improvement in Coincidence Time Resolution (CTR) from 28.86 ps to 18.44 ps.



*Comparison of scintillation kinetics between standard (left) and GAGG:Ce. Mg (right) incorporation eliminates shallow trap-mediated slow decay by suppressing $Gd_{Al}$ defects and enables fast direct capture at $Ce^{4+}$ centers, while deep traps $Gd_{Al}$−VO introduce non-radiative quenching pathways.*

This study provides a unified theoretical framework linking defect engineering to macroscopic scintillator performance.

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