

Spectroscopic calculations for trivalent lanthanide ions

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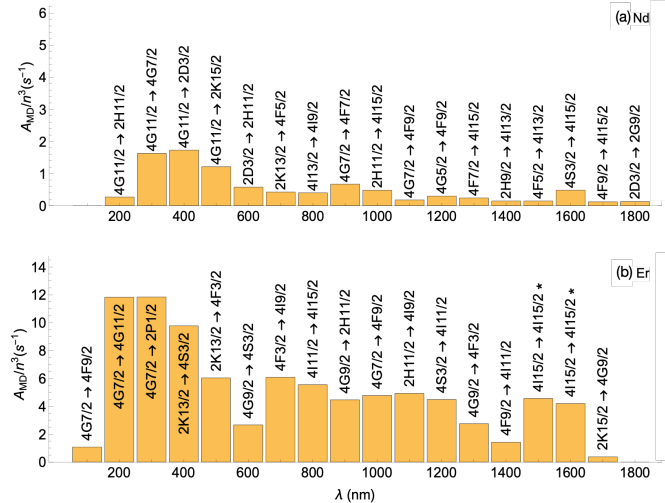
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It has been shown that the spin of optically addressable solid-state defects can be coherently manipulated using electric fields [1,2], enabling precise control over the photoluminescence spectra of spin defects when integrated into electrical junctions. Additionally, spin defects are also sensitive to electric and magnetic field noise [3], for instance, electric field noise from surface charge fluctuations can be a significant source of spin decoherence [4].

In this study, we examine trivalent lanthanide ion defects in crystals using a semi-empirical Hamiltonian, where parameters are empirically fitted to experimental data. By diagonalizing the Hamiltonian, we are able to predict key spectroscopic properties of these defects, including optical transition rates, oscillator strengths, magnetic dipole transitions, parity-



forbidden electric dipole transitions, AC Stark shifts, and g-tensors for low-energy excitations. We have compared our results against the well-established calculations from Carnall et al. [5], for the lanthanide ions in LaF₃ and make available the *qlanth* software for easy reproducibility of the results. These findings are essential for advancing the control of rare-earth-based quantum devices and for understanding the mechanisms underlying their decoherence.

Figure 1. Maximum emission rate, due to magnetic dipole, of Nd³⁺ and Er³⁺ in LaF₃ within a frequency window, labelled by the main (2S+1)LJ component of the initial and final state.

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