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First-principles identification of optically active Er^{3+} centers in GaN KHANG HOANG, North Dakota State University — Rare-earth (RE) doped III-nitrides are of great interest for optoelectronic and spintronic applications. The identification of optically active RE centers in these materials has however been challenging, both in experimental and theoretical/computational studies. In this talk, we present a hybrid density functional study of the interaction between the erbium (Er) dopant and wurtzite GaN, including intrinsic point defects and other impurities that may be present in the host material. Particularly, we investigate the structure, energetics, and transition levels of the Er impurity and its complexes with N and Ga vacancies, substitutional C and O impurities, and H interstitials. In light of our results, we identify possible luminescent Er^{3+} centers in Er-doped GaN and discuss the role of these centers in the excitation of the Er $4f$-electron core.

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