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Accurate first-principles calculation of the rare earth crystal field FEI ZHOU, VIDVUDS OZOLINS, UCLA — Rare earth (RE) doped wide band-gap semiconductors play an important role in solid state lighting. Many aspects of the performance of these materials are characterized and determined by the f-electron crystal field (CF). However, CF effects are usually rather small for f electron: the CF splitting is at the order of 0.1 eV, compared to several eV for d-electrons. Therefore accurate theoretical description of RE crystal field is challenging. We present a first-principles method of CF calculation based on an improved LDA+U method. By careful cancellation of errors, the method can reach relatively high accuracy for the CF parameters. As a demonstration we calculate the experimentally well-characterized RE:LaF_3 system, which has low point-group symmetry and a large number of CF parameters, representing a stringent test of theory. The predicted CF excitation energies of Ce:LaF3 agree within about 10 meV with experiment, and within several meV if the errors in the free-ion parameters are excluded. Work is underway to apply the method to other materials for solid-state lighting and laser applications.

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