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Correlation effects in La, Ce, and lanthanide ions CHARLES W. CLARK, Joint Quantum Institute, NIST and the University of Maryland, MARIANNA SAFRONOVA, University of Delaware and JQI, NIST and the University of Maryland, ULYANA SAFRONOVA, University of Nevada, Reno — We carry out a comprehensive study of higher-order correlation effects to the excitation energies of La, La^+, Ce, Ce^+, Ce^{2+}, and Ce^{3+}. The calculations are carried out using two hybrid approaches that combine configuration interaction with second-order perturbation theory and the linearized coupled-cluster all-order method. Use of two approaches allows us to isolate the effects of third- and higher-order corrections for various configurations. Comparison of results for monovalent and multivalent systems allowed us to separately study the importance of the core-valence and valence-valence correction. We also study the contribution of higher partial waves and investigate methods to extrapolate the effect of omitted partial waves. The effects of the higher partial waves for the monovalent configuration of La^{2+} and Ce^{3+} are compared with analogous effects in multivalent configurations of La, La^+, Ce, Ce^+, and Ce^{2+}. Tests of our extrapolation techniques are carried out for several Cd-like lanthanide ions. The results of the present studies are of particular interest to the development of high-precision methods for treatment of systems with partially filled nf shells that are of current experimental interest for a diverse set of applications.

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