Title:	Potential Energy Curves of Molecular Nitrogen for Singly and Doubly Ionized States with Core and Valence Holes
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Abstract:	Theoretical description of potential energy curves (PECs) of molecular ions is essential for interpretation and prediction of coupled electron-nuclear dynamics following ionization of parent molecule. However, an accurate representation of these PECs for core or inner valence ionized state is nontrivial, especially at stretched geometries for double- or triple-bonded systems. In this work, we report PECs of singly and doubly ionized states of molecular nitrogen using state-of-the-art quantum chemical methods. The valence, inner valence, and core ionized states have been computed. A double-loop optimization scheme that separates the treatment of the core and the valence orbitals during the orbital optimization step of the multiconfiguration self-consistent field method has been implemented. This technique allows the energy to be converged to any desired ionized state with any number of core or inner-shell holes. The present work also compares the PECs obtained using both delocalized and localized sets of orbitals for the core hole states. The PECs of a number of singly and doubly ionized valence states have also been computed and compared with previous studies. The computed PECs reported here are expected to be of importance for future studies to understand the interplay between photoionization and Auger spectra during the breakup of molecular nitrogen when interacting with intense free electron lasers.
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