

Abstract Submitted
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Coupled-cluster methods for core-hole dynamics¹ ANTONIO PICON, Argonne National Laboratory, LAN CHENG, The University of Texas at Austin, JEFF R. HAMMOND, Argonne National Laboratory, JOHN F. STANTON, The University of Texas at Austin, STEPHEN H. SOUTHWORTH, Argonne National Laboratory — Coupled cluster (CC) is a powerful numerical method used in quantum chemistry in order to take into account electron correlation with high accuracy and size consistency. In the CC framework, excited, ionized, and electron-attached states can be described by the equation of motion (EOM) CC technique. However, bringing CC methods to describe molecular dynamics induced by x rays is challenging. X rays have the special feature of interacting with core-shell electrons that are close to the nucleus. Core-shell electrons can be ionized or excited to a valence shell, leaving a core-hole that will decay very fast (e.g. 2.4 fs for K-shell of Ne) by emitting photons (fluorescence process) or electrons (Auger process). Both processes are a clear manifestation of a many-body effect, involving electrons in the continuum in the case of Auger processes. We review our progress of developing EOM-CC methods for core-hole dynamics. Results of the calculations will be compared with measurements on core-hole decays in atomic Xe and molecular XeF₂.

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