Photoionization of confined noble gas atoms: Hybridization and interchannel coupling effects

MOHAMMAD JAVANI, Georgia State University, HIMADRI S. CHAKRABORTY, Northwest Missouri State University, STEVEN T. MANSON, Georgia State University — A theoretical study of the photoionization of the noble gas atoms Ne, Ar, Kr and Xe confined endohedrally with a C\textsubscript{60} fullerene molecule is presented. The fullerene shell is represented by a jellium potential of 60 smeared out C\textsuperscript{4+} ions and the wave functions 240 delocalized valence electrons plus the atomic electrons move in the field generated by the atomic potential plus the shell potential. The photoionization is calculated within the framework of the time-dependent local-density approximation (TDLDA) \cite{1} which includes significant aspects of correlation. The results show that in all four cases, the valence photoionization channel cross sections of the entrapped atoms are dramatically increased by interchannel coupling with the C\textsubscript{60} plasmons. In addition, hybridization, the mixing of initial-state wave functions of atom and shell, occurs in a number of cases, a phenomenon which substantially alters the cross sections of both the atomic and the shell states. Confinement resonances are also in evidence for all cases. The evolution of these effects along the noble gas sequence is discussed.

\cite{1} M.E. Madjet et al., \textit{Phys. Rev. A} \textbf{81}, 013202 (2010).

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