Modeling A@C\textsubscript{60} atoms: diffuse versus square-well confining pseudo-potentials\textsuperscript{1} JONATHAN KING, JOSHUA OGLESBY, VALERIY DOLMATOV, University of North Alabama — An empirical model approximating the C\textsubscript{60} cage potential by a square-well confining potential has played an important role in providing the initial understanding of photoionization spectra of A@C\textsubscript{60} endohedral atoms \cite{1}. However, the square-well potential is discontinuous at its boarders. A more realistic confining potential must be diffuse, obviously. However, it is not at all clear \textit{apriori} to what degree replacement of a square-well potential by a diffuse potential may alter predictability of the model. In particular, should a large array of predicted data and phenomena made on the basis of a square-well potential model be re-studied with an eye on a more realistic diffuse potential boarders of C\textsubscript{60}? It will be shown in this presentation, with H@C\textsubscript{60} and Xe@C\textsubscript{60} as case studies, that both the square-well and diffuse confining potentials lead to practically identical calculated data for A@C\textsubscript{60} photoionization spectra. Moreover, the latter are largely insensitive to the degree of diffuseness of the potential, in reasonable limits. Hence, either of said potentials is equally suitable for mimicking the C\textsubscript{60} cage.

\textsuperscript{1}This work was supported by the RUI NSF grant No. PHY-0969386.