

Abstract Submitted  
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**Modeling A@C<sub>60</sub> atoms: diffuse versus square-well confining pseudo-potentials**<sup>1</sup> JONATHAN KING, JOSHUA OGLESBY, VALERIY DOLMATOV, University of North Alabama — An empirical model approximating the C<sub>60</sub> cage potential by a square-well confining potential has played an important role in providing the initial understanding of photoionization spectra of A@C<sub>60</sub> endohedral atoms [1]. However, the square-well potential is discontinuous at its borders. A more realistic confining potential must be diffuse, obviously. However, it is not at all clear *a priori* 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 borders of C<sub>60</sub>? It will be shown in this presentation, with H@C<sub>60</sub> and Xe@C<sub>60</sub> as case studies, that both the square-well and diffuse confining potentials lead to practically identical calculated data for A@C<sub>60</sub> 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<sub>60</sub> cage.

[1] V. K. Dolmatov, Adv. Quant. Chem. **58**, 13 (2009).

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