$e + \mathrm{C}_{60}$ and $e + A@\mathrm{C}_{60}$ elastic scattering versus the parameters of the C_{60}-model-square-well potential

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Synopsis Modelling of the C_{60} cage by a square-well potential $U_\mathrm{c}(r)$ is a popular approximation. In the literature, some inconsistency is present in choosing the magnitudes of parameters of $U_\mathrm{c}(r)$. In the present study, $e+\mathrm{C}_{60}$ and $e + A@\mathrm{C}_{60}$ elastic scattering is scrutinized versus the parameters of $U_\mathrm{c}(r)$ in order to identify $U_\mathrm{c}(r)$ which is best suited for studying *electron-fullerene* scattering and how the latter can be controlled by tuning the potential.

The work [1] demonstrated a reasonable usability of modelling the C_{60} cage by an attractive square-well (in the radial coordinate) potential $U_\mathrm{c}(r)$ for the study of $e + \mathrm{C}_{60}$ elastic scattering. This is because the most prominent features of $e + \mathrm{C}_{60}$ scattering, predicted by the model [figure 1(a), solid line], agree qualitatively and even semi-quantitatively with calculated data obtained in the framework of a sophisticated *ab initio* molecular-Hartree-Fock (MHF) approximation [figure 1(a), dash line] [1]. Later [2], the model was applied to $e+A@\mathrm{C}_{60}$ elastic scattering as well. In [1, 2], $U_\mathrm{c}(r)$ [to be labelled as $U_{1\mathrm{c}}(r)$ in the paper] was defined as follows (in atomic units): the width $\Delta = 2.9102$, the inner radius $R_0 = 5.262$, the depth $U_0 = 0.2599$. The binding strength of $U_{1\mathrm{c}}(r)$ (into a 2p state) matches the electron affinity of C_{60}, $EA = -2.65$ eV. However, in the literature, square-well potentials with other magnitudes of the parameters but the same binding strength as $U_{1\mathrm{c}}(r)$ are used as well: $U_{2c}(r)$ with $R_0 = 5.8$, $\Delta = 1.9$, $U_0 = 0.302$ [3] and $U_{3\mathrm{c}}(r)$ with $R_0 = 6.01$, $\Delta = 1.25$ and $U_0 = 0.422$ [4] (their binding strength matches the electron affinity of C_{60} relative to the 1s state). It is the ultimate aim of the present study (a) to clarify which one of these potentials is best suited for studying *electron-fullerene* scattering and (b) to learn how *electron-fullerene* scattering could be controlled by tuning the parameters of $U_\mathrm{c}(r)$. The latter is an interesting in and of itself study from a point of view of basic science. Calculated electron elastic scattering cross sections $\sigma_\mathrm{el}^{\mathrm{C}_{60}}$ and $\sigma_\mathrm{el}^{Ba@\mathrm{C}_{60}}$ are depicted in figure 1. The results identify how, in principle, parameters of the resonances seen in $\sigma_\mathrm{el}^{\mathrm{C}_{60}}$ and $\sigma_\mathrm{el}^{Ba@\mathrm{C}_{60}}$, as well as even the very existence of some of them, can be modified by changing parameters of $U_\mathrm{c}(r)$. Furthermore, results, obtained with the use of the potentials $U_{2\mathrm{c}}$ and $U_{3\mathrm{c}}$, appear to differ noticeably from data calculated both with the use of $U_{1\mathrm{c}}$ and in *ab initio* MHF. Thus, the potential

$U_{1\mathrm{c}}$ is a better potential than $U_{2\mathrm{c}}$ and $U_{3\mathrm{c}}$ for the study of *electron-fullerene* scattering, providing that MHF serves as the reference approximation.
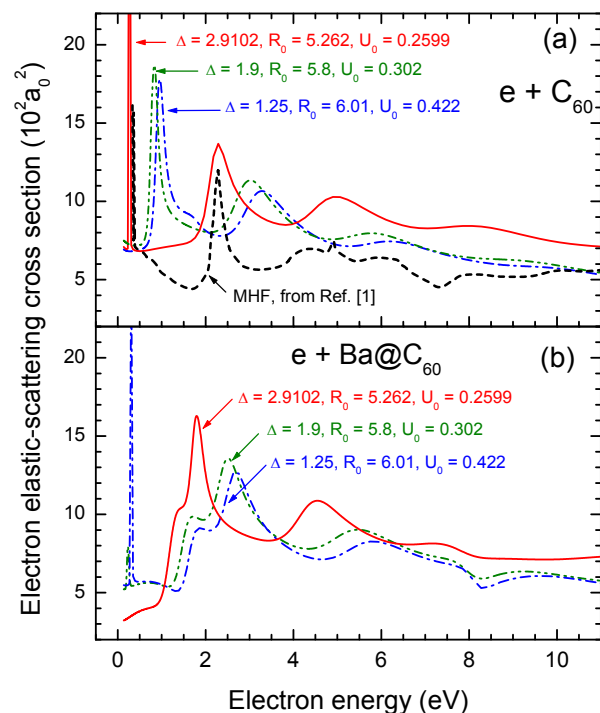

Figure 1. Electron elastic scattering cross sections $\sigma_\mathrm{el}^{\mathrm{C}_{60}}$ and $\sigma_\mathrm{el}^{Ba@\mathrm{C}_{60}}$ calculated with the use of different square-well potentials matching the electron affinity of C_{60}, $EA = -2.65$ eV, as well as $\sigma_\mathrm{el}^{\mathrm{C}_{60}}$ calculated in *ab initio* MHF [1], as marked.

References

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