Electron elastic scattering off $A@C_{60}$ fullerenes: the “zeroth-order” trends$^1$ M. HUNTER, M. COOPER, C. BAYENS, V. DOLMATOV, University of North Alabama — The theoretically revealed trends in electron elastic scattering off endohedral fullerenes $A@C_{60}$ associated with the nature of an encapsulated atom $A$, its size and spin ($A = \text{Ar, Xe, Ba, Cr and Mn}$) are highlighted. It is shown that placing an atom $A$ inside the $C_{60}$ cage can make electron scattering off $A@C_{60}$ weaker than off the empty $C_{60}$ cage, especially when the encapsulated atom $A$ donates an appreciable part of its electron density to the $C_{60}$ cage, as do Ba, Cr and Mn. It is shown that, for such atoms, $e + A@C_{60}$ scattering can even be weaker than off the isolated atom A itself. In addition, if such encapsulated atom has also a nonzero spin $S$ (Cr’s $S = 3$, Mn’s $S = 5/2$), then the $C_{60}$ cage can become “spin-charged”; this results in a strong electron spin-dependence of $e + A@C_{60}$ scattering. In calculations, (a) electron correlation was ignored, (b) both the encapsulated atom $A$ and $C_{60}$ cage were regarded as non-polarizable targets, and (c) the $C_{60}$ cage was modeled by a spherical annular well. Results, thus, provide the understanding of $e + A@C_{60}$ scattering in a “zeroth-order” approximation and, most likely, identify some of the most intrinsic properties of $e + A@C_{60}$ elastic scattering.

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