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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 = 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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