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Non-perturbative treatment of orange-type potential in endohedrals MIRON YA. AMUSIA, Racah Institute of Physics, Hebrew University, Jerusalem, Israel and Ioffe Physico-Technical Institute, St. Petersburg, Russia, LARISSA V. CHERNYSHEVA, Ioffe Physico-Technical Institute, St. Petersburg, Russia — We developed a system of programs that permit to treat non-perturbatively the effect of the fullerene shell upon the stuffed atom photoelectrons in the frame of RPAE. We use the zero-thickness “orange-skin” potential. Usually this potential was applied to calculate a factor that permitted to obtain all photoionization characteristics of an endohedral directly from respective characteristics of isolated atoms. It appeared, however that even when the photoelectron energy is low enough, the fullerenes shell can affect not only the real states of the electron on the way of the atom. Surprisingly enough at the first glance, the fullerene shell, even being remote quite far from the central atom in the endohedral, can strongly affect the intermediate virtual states. Therefore, the factorization of the fullerenes shell effects become in general incorrect. To take the modification of the virtual states, one has to treat the considered process with participation of the endohedral atom within the frame of a given model. We developed simple programs that permit to take into account one zero-thickness fullerenes potential or two – for “onion-type” endohedrals in the RPAE frame and performed concrete calculations for Ar@C60.

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