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Photoionization of Molecular Endohedrals. MIRON AMUSIA, Hebrew Univ of Jerusalem; Ioffe Phys-Tech. Institute, LARISSA CHERNYSHEVA, Ioffe Phys-Tech. Institute, SERGEY SEMENOV, Retired — We calculate the photoionization cross-section of a molecular endohedral $M@C_N$. We limit ourselves to two-atomic molecules. The consideration is much more complex than for atomic endohedrals because the system even for almost spherical C_N has only cylindrical instead of spherical symmetry. But $M@C_N$ is more interesting since the interelectron interaction in molecules is relatively stronger than in similar atoms. We present results of calculations of molecular hydrogen H_2 stuffed inside almost spherical fullerene C_{60} – $H_2@C_{60}$. For comparison, we perform calculations also for atomic endohedral $He@C_{60}$. The results are obtained both in single-electron Hartree-Fock approximation and with account of multi-electron correlations in the frame of so-called random phase approximation with exchange – RPAE. The presence of the fullerenes shell results in prominent oscillations in the endohedrals photoionization cross section. The role of interelectron correlations becomes clear by comparing HF and RPAE results for $H_2@C_{60}$ and $He@C_{60}$ on the one side with that for H_2 and He, on the other.

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