Open-shell molecule: Problems of computer simulation and the reality of spin contamination of the molecule ground state

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Open-shell molecules belong to atomic systems with a considerable electron correlation. Close-to-degeneracy electron states strongly influence the spin symmetry consideration due to which complicated schemes related to configurational interaction (CI) are needed to provide appropriate computer simulations of the species. The paper presents one of possible ways to tackle the problem by using CI bi-determinant Hartree-Fock approximation. A particular attention is given to spin-contamination of the states that is a distinguishing characteristic of the electron correlation at any level of the theory. Basing on results obtained for graphene molecules and addressing the available experimental data allow for suggesting that the spin contamination of the ground state of open-shell molecules is a physical reality.