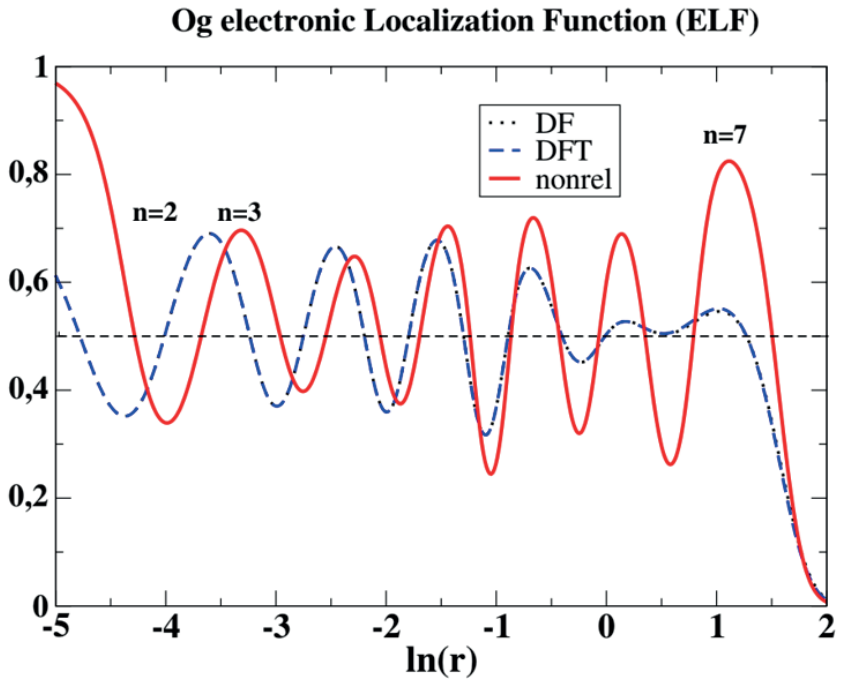
LOCALIZATION OF ELECTRON STATES OF OGANESSON ATOM

Tupitsyn I.I., Kaygorodov M.Y., Shabaev V.M.

St.Petersburg State University, Universitetskaya nab. 7/9, St.Petersburg, 199034, Russia,
e-mail: v.shabaev@spbu.ru

In Ref.[1] it was claimed that the large relativistic effects in the oganesson atom, ^{294}Og (Z = 118), smear out valence one-particle density, thus making it approaching the electron-gas regime. This conclusion was made using the analysis of electronic localization function (0 <ELF <1), which was introduced in quantum chemistry in Ref.[2]. For highly localized electron states on atomic shells ELF is close to 1 and ELF=0.5 for a uniform electron gas (see Fig.). In the case of zero electron density the ELF value is close to zero.



In the present work, we performed calculations of various quantities that characterize the degree of localization of valence wave functions and smearing of the valence shells. The Hartree-Fock method was used to calculate relativistic and non-relativistic ELFs, and the root mean square radii and standard deviations of the wave functions. The population of atomic orbitals and other quantities were calculated using the configuration interaction method. On the basis of the calculations performed, a conclusion was made that despite the fact that the ELF value in the valence region in the relativistic case is close to 0.5 (see Fig.), the structure of atomic valence shells is preserved and the electron density distribution does not correspond to free electron gas.

References
1. Jerabek, P., et al., Phys. Rev. Lett. 2018, 120, 053001.
2. Becke, A.D.; Edgecombe, K.E., J. Chem. Phys. 1990, 92, 5397.