DENSITY FUNCTIONAL THEORY IN ATOMIC PHYSICS

E.S. Kryachko[1], *E.Yu. Remeta*[2]

[1]Bogolyubov Institute for Theoretical Physics,
Nat. Acad. of Sci. of Ukraine
(*14b, Metrolohichna Str., Kyiv 03143, Ukraine*)
[2]Institute of Electron Physics,
Nat. Acad. of Sci. of Ukraine
(*21, Universitetska Str., Uzhgorod 88017, Ukraine*)

S u m m a r y

We offer a broad range of issues lying at the heart of density functional theory, DFT, which is currently omnipresent in nearly all computational studies of atoms, molecules, solids, and nano-materials and composes the grounds of modern many-body computational techiques. A key goal of this review is twofold. First, on the basis of the studies of properties of atomic systems, to present all "pros and cons" of the standard DFT that originated from the Hohenberg–Kohn theorem and the self-consistent Kohn–Sham field theory. Second, to show the ways of its improval, basically relaying on the method of local-scaling transformations where the one-electron density plays, as should be within the DFT context, a natural role of variable.