

Abstract Submitted
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Internal inconsistency of Kohn-Sham equations in density-functional-theory¹ BOYAN OBRESHKOV — The conflict of DFT Kohn-Sham equations with the Ritz variational principle will be demonstrated rigorously. It will be shown that the ground-state charge density of the material is not representable by auxiliary one-electron orbitals of variational character. This inconsistency is also expressed by a charge-sloshing effect in attempt to solve these equations self-consistently.

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