Quantal Density Functional Theory

Quantal density functional theory (Q-DFT) is a new local effective potential energy theory of the electronic structure of matter. It is a description in terms of classical fields that pervade all space, and their quantal sources. The fields, which are explicitly defined, are separately representative of the many-body electron correlations present in such a description, namely, those due to the Pauli exclusion principle, Coulomb repulsion, correlation-kinetic, and correlation-current-density effects. The book further describes Schrödinger theory from the new perspective of fields and quantal sources. It also explains the physics underlying the functionals and functional derivatives of traditional DFT.

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Kundenservice Fachmedien Otto Schmidt Neumannstraße 10, 40235 Düsseldorf | <u>kundenservice@fachmedien.de</u> | 0800 000-1637 (Inland)

