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Density Functional Resonance Theory: The Complex Density Function, Orbital Energies and Lifetimes, and Results for Simple Systems[1] DANIEL WHITENACK, Purdue University Department of Physics, ADAM WASSERMAN, Purdue University Department of Chemistry and Department of Physics — Density Functional Resonance Theory (DFRT) is a recently developed complex-scaled version of ground-state Density Functional Theory (DFT) for metastable systems. This work is a detailed study of the formalism itself, its consequences and its application. The meaning of the complex "density" function, which is used as the primary variable, is discussed along with its possible application to study the reactivity of metastable systems. In addition, orbital energies and lifetimes are defined and related to physical quantities. Finally, results for energies and lifetimes are presented for simple systems.

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Daniel Whitenack
Purdue University Department of Physics

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