

# New Algebraic Formulation of *Ab Initio* Calculation: DFT++

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This talk addresses a fundamental problem faced by the *ab initio* community: the lack of an effective formalism for the rapid exploration and exchange of new methods. To rectify this, we introduce a new formulation which for density-functional theory is what the Dirac notation is for quantum mechanics: a language free of burdensome details which permits the ready performance of complex manipulations with focus on physical content.

This new, basis-set independent, matrix-based formulation reduces the development, implementation, and dissemination of new *ab initio* techniques to the derivation and transcription of a few lines of algebra. We believe that this framework would be a boon to the community were it to adopt it. We conclude with a presentation of our strategies for optimization and parallelization, their ease of implementation, and the resulting computational performance.