

# Project Proposal: DFT++ through Genetic Optimization

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## Abstract

I intend to implement a small DFT++ code in MATLAB using a novel optimization algorithm [1]. DFT++ is an alternate formulation of density functional theory in which the Kohn-Sham equations are expressed as an optimization problem [4]. This optimization step is the most computationally expensive part of the approach.

In an attempt to accelerate convergence, we will perform the necessary optimizations using a genetic algorithm. The essential genetic information on which we will be acting is the charge density itself. That is, two trial solutions to the energy minimization problem will be two different charge densities. Evaluating the fitness of trial solutions is easily done by total energy calculation. We must also develop a crossover operation in which we combine two “parent” two solutions into an “offspring” solution, maintaining what is good about the electronic structure of the parents. To this end, we can exploit the partial spatial separability of the energy-minimisation problem: two chunks of nearby electronic density interact more importantly than more distant chunks. So, a crossover operator could take a slice or slab of the density from each parent and slap them together to make a child. Similar strategies have been applied to the ab-initio structure prediction problem [5],[2],[3].

Through this work, I will gain a deeper understanding of the theoretical underpinnings as well as the practical implementation of a density functional theory code. I will learn more about a powerful, modern optimization technique and hopefully make an improvement on a current method of performing electronic structure calculations. Finally, I will present my code as well as calculations on trial systems which I will verify using traditional DFT calculations.

## References

- [1] Tomas Arias. Dft++ minicourse. <http://dft.physics.cornell.edu/minicourse/>.
- [2] D. M. Deaven. Molecular geometry optimization with a genetic algorithm. *Physical Review Letters*, 75, 1995.
- [3] Colin W. Glass. Uspex—evolutionary crystal structure prediction. *Computer Physics Communications*, 175, 2006.
- [4] Sohrab Ismail-Beigi and T. A. Arias. New algebraic formulation of density functional calculation. *Computer Physics Communications*, 128:1, 2000.
- [5] Giancarlo Trimarchi. Global space-group optimization problem: Finding the stablest crystal structure without constraints. *Physical Review B*, 75, 2007.