Maldon Owen Physics Prize 2025

This award (of £250) is given to the best graduating student on an M Phys programme at the University of York

Winner: Kit Brown

Title:

Using Bosonic Density Functional Theory To Accelerate Finite Displacement Calculations

Description:

Density functional theory (DFT) is a method of ab initio materials modelling using the electronic density, rather than a wavefunction to describe the system. Kohn-Sham DFT uses an auxiliary system of noninteracting fermionic particles to model the real system for improved accuracy in calculation of the kinetic energy over functional-based approximations. This auxiliary system requires the orthogonalisation of single particle states to mimic the behaviour of the Pauli exclusion principle. Using computational methods to orthogonalise N single particle states has a cost of O(N3) in time and O(N2) in memory. Alternative auxiliary systems of non-interacting bosonic particles were investigated with the goal of accelerating finite displacement calculations. This family of calculations are commonly used to calculate properties of materials relevant to problems such as heat dissipation and electrical conductivity. A bosonic auxiliary system is shown to speed up DFT calculations given a target density to determine the bosonic Kohn-Sham potential. Initial attempts at approximating the bosonic potential via a perturbation of the external potential are shown to be insufficient for accurate phonon calculations. These results demonstrate that time savings are possible with the use of bosonic calculations, however further work is needed to find accurate approximations to the bosonic Kohn-Sham potential.