ABSTRACT

THESIS: TESTING ORBITAL FREE MODELS OF THE KINETIC ENERGY DENSITY IN SEMICONDUCTORS

STUDENT: AKINFOLARIN AKINOLA

DEGREE: MASTER OF SCIENCE

COLLEGE: SCIENCE AND HUMANITIES

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Kohn-Sham (KS) density functional theory (DFT) is the most used method of electronic structure calculations because of its accuracy and computational cost efficiency at predicting the structural properties of materials. The difficult term to treat in the KS energy functional is the non-classical many-body contribution to energy, the exchange-correlation (XC) energy. This must be approximated. Meta-generalized gradient approximations (mGGAs) are a class of XC models conventionally dependent on the electron density, density gradient, and KS kinetic energy density (KED). The addition of the KED makes mGGAs accurate for predicting structural properties but also computationally expensive for some applications such as ab initio molecular dynamics. This computational bottleneck arises due to the use of orbitals for each independent particle to get accurate KED. Our goal is to determine how well the exact KED can be represented by a single mGGA model in terms of density, dimensionless density gradient, and dimensionless density Laplacian. In prior research, our group calculated the exact KED and density of semiconductor solids with varying ionicity and atomic number using the ABINIT DFT plane-wave pseudopotential code. The current work tests how orbital-free models for the KE perform compare to exact KS

results for important structural properties for our test set of semiconductors. We calculate the energy for each material at a variety of lattice constants. A fit to the Stabilized Jellium or Murnaghan equation of state is used to obtain structural parameters. We calculate the exact KE and orbital-free models for each data set to obtain the change in KE and total energy for that model. We develop and test new orbital free models for the KED based on known exact behavior for the limit of slowly varying density and fitting to the semiconductor data.