

# Self consistent charge and dipole density functional tight binding method and its application to carbon-based systems

Ying Wu<sup>a,b</sup>, Adelina Ilie<sup>a,b</sup> and Simon Crampin<sup>a,b</sup>

<sup>a</sup> Department of Physics, University of Bath, Bath BA2 7AY, United Kingdom

<sup>b</sup> Centre for Graphene science, University of Bath, Bath BA2 7AY, United Kingdom

[y.wu@bath.ac.uk](mailto:y.wu@bath.ac.uk)

## Abstract

The density functional tight binding (DFTB) method is a fast, semi-empirical, total energy electronic structure method based upon and parameterized to density functional theory (DFT). The standard self-consistent charge (SCC) DFTB approximates the charge fluctuations in a system using a multipole expansion truncated to the monopole term [1,2]. For systems with asymmetric charge distributions, such as might be induced by an applied external field, higher terms in the multipole expansion are likely to be important. We have extended the formalism to include dipoles (SCC+D), have implemented the method computationally, and tested it by calculating the response of various carbon nanotubes and fullerenes to an applied electric field. A comparison of polarizabilities with experimental data or more sophisticated DFT calculations indicates a substantial improvement over standard SCC-DFTB. We also discuss the issues surrounding parameterization of the new SCC+D DFTB scheme.

## References

- [1] M. Elstner, et. al, Phys. Rev. B, **58** (1998) 7260.
- [2] Z. Bodrog, et. al, Phys. Status. Solidi B, **249** (2012) 259.