

DISPERSION CORRECTIONS IN DENSITY FIELD THEORY

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Abstract

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CONTENTS	§ 3.	PURE METHODS
1. INTRODUCTION	I	VV _{IO} , vdW-DFT
2. EMPIRICALLY BASED METHODS	I	
2.1 DFT-D ₂	I	
3. PURE METHODS	I	

§ 1. INTRODUCTION

Covalent and ionic bonds are normally considered the most important interactions in terms of making a molecule, but the lesser known dispersion interaction (often known as Van der Waals interactions, or London Dispersion forces) plays just as an important role, if not more so in some highly important molecules like DNA. Primitive DFT methods neglected these interactions, causing DNA to unwind and benzene rings to repel each other. Whilst this wasn't as much a problem in basic solid state physics, where unit cells are only made up of purely covalent or ionic bonds, it affects all areas of science where complicated molecules are involved. Many diverse solutions were developed, and are still being developed today, to overcome this problem. They include methods which are fit to empirical data, like Grimme's DFT-D₂ and DFT-D₃, which are generally faster. And pure methods, such as VV_{IO} and vdW-DFT, which are much more costly.

§ 2. EMPIRICALLY BASED METHODS

§ 2.1. **DFT-D₂.** In 2006 Stefan Grimme released DFT-D₂[1], the successor to his more limited DFT-D method. The basis of DFT-D₂ is in pairwise attraction between atoms, however, it doesn't take into account its chemical environment, see: DFT-D₃. Despite being less accurate than D₃, D₂ is still widely used due to its relatively high accuracy and low cost.

REFERENCES

- [1] S. Grimme, 'Semiempirical gga-type density functional constructed with a long-range dispersion correction,' *Journal of Computational Chemistry*, vol. 27, no. 15, pp. 1787–1799, 2006. doi: <https://doi.org/10.1002/jcc.20495>. eprint: <https://onlinelibrary.wiley.com/doi/pdf/10.1002/jcc.20495>. [Online]. Available: <https://onlinelibrary.wiley.com/doi/abs/10.1002/jcc.20495>.