

# DISPERSION CORRECTIONS IN DENSITY FIELD THEORY

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## Abstract

Fusce mauris. Vestibulum luctus nibh at lectus. Sed bibendum, nulla a faucibus semper, leo velit ultricies tellus, ac venenatis arcu wisi vel nisl. Vestibulum diam. Aliquam pellentesque, augue quis sagittis posuere, turpis lacus congue quam, in hendrerit risus eros eget felis. Maecenas eget erat in sapien mattis porttitor. Vestibulum porttitor. Nulla facilisi. Sed a turpis eu lacus commodo facilisis. Morbi fringilla, wisi in dignissim interdum, justo lectus sagittis dui, et vehicula libero dui cursus dui. Mauris tempor ligula sed lacus. Duis cursus enim ut augue. Cras ac magna. Cras nulla. Nulla egestas. Curabitur a leo. Quisque egestas wisi eget nunc. Nam feugiat lacus vel est. Curabitur consectetur.

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## § 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-D<sub>2</sub> and DFT-D<sub>3</sub>, which are generally faster. And pure methods, such as VV<sub>IO</sub> and vdW-DFT, which are much more costly.

## § 2. EMPIRICALLY BASED METHODS

§ 2.1. **DFT-D<sub>2</sub>.** In 2006 Stefan Grimme published DFT-D<sub>2</sub>[1], the successor to his more limited DFT-D method. The basis of DFT-D<sub>2</sub> is in pairwise attraction between atoms, however, it doesn't take into account its chemical environment, see: DFT-D<sub>3</sub>. Despite being less accurate than D<sub>3</sub>, D<sub>2</sub> 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>.