Density Functional Theory Including van der Waals Forces

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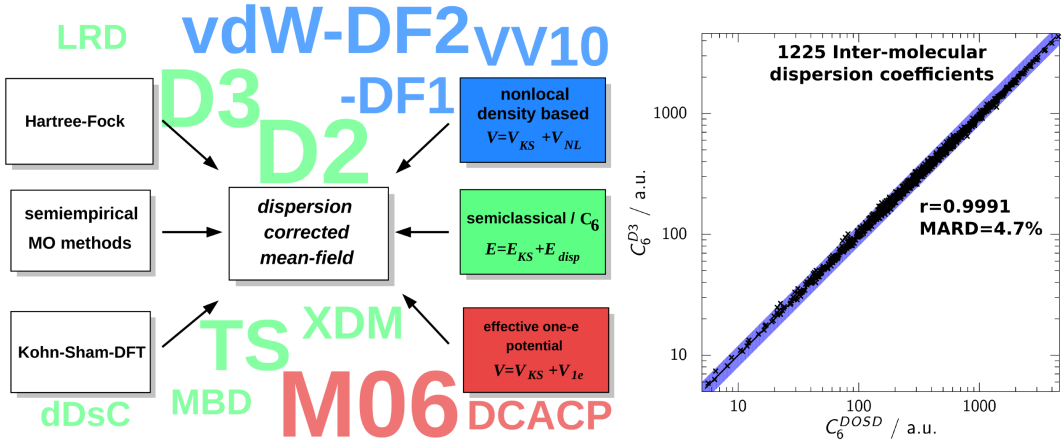
In the past years we have learned that good structures are the key to many important physical and chemical properties. In the foreseeable future, Kohn-Sham density functional approximations (DFA) will continue to be the method of choice for geometry optimizations. I will present different ways to incorporate London dispersion interactions (attractive van der Waals forces) in the density functional framework. They are classified into nonlocal (density based), semi-classical (C_6 based), and effective one-electron potentials.[1]
Those correction schemes can be ideally combined with semi-local DFAs to generate highly accurate electronic structure methods. As an example, a new cost-efficient screened exchange hybrid functional HSE-3c, which is targeting molecular crystals and their property prediction will be introduced.[2, 3] Comprehensive benchmark results show the overall accuracy of different approaches, where the impact of dispersion interactions is highlighted. I will demonstrate the application of some discussed methods to the 6^{th} blind test for organic crystal structure prediction. Comparisons to other state-of-the-art methods indicate both problems and success in the recent method developments.[4, 5]



Key references

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