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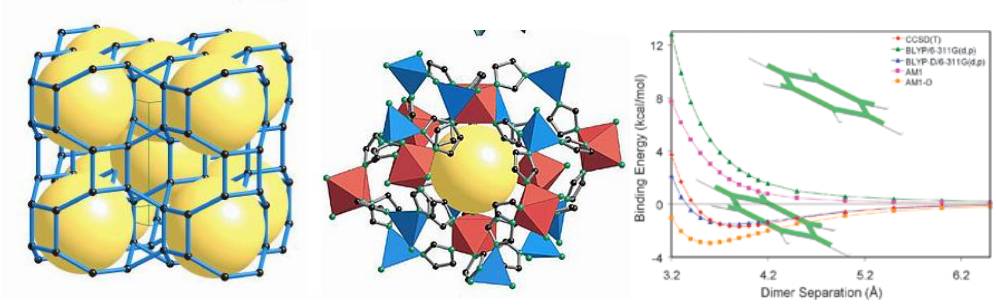
VAN DER WAALS PARAMETERS FOR HOST-GUEST INTERACTIONS IN NANOPOROUS MATERIALS

Keywords: host-guest interactions, model development, dispersion

Molecular recognition and host-guest interactions play a key role in a variety of chemical and biological processes including chemical sensing, drug delivery, chemical and enzymatic catalysis, and chemical separations. In particular nanoporous materials are very promising for a variety of applications due to their high surface to volume ratio. They can virtually act as molecular sponges for carbon dioxide capture, hydrogen storage,… They have pores within the 0.2 to 50 nm range and can act as a host for various small molecules. The accurate description of such host-guest interactions is very challenging from theoretical point of view as it concerns long-range dispersion interaction which act between molecules even in the absence of charges or permanent electric moments. They stem from many-particle (electron-correlation) effects that are complicated by the quantum-mechanical wave-nature of matter. Only very advanced ab initio correlated wavefunction methods are able to account for these effects but are computationally too demanding for routine studies in larger molecular systems. Density functional theory (DFT) is now the most widely used method for electronic structure calculations in condensed matter physics and quantum chemistry. This success mainly results from significant 'robustness', i.e. providing reasonable accurate predictions for many properties of various molecules and solids at affordable computational expense. However, a general drawback of all common density functionals is that they can not describe long-range electrostatic correlations that are responsible for the dispersion forces. The DFT problem for vdW interactions now has become a very active field of research and recently several solutions were proposed. From a practical point of view, where the focus is on robustness and computational speed, empirical –C6R-6 corrections to standard density functionals seem most promising. This is called the DFT-D approach and provides high accuracy in many different situations.



Goal For nanoporous materials with transition metals the validity of the DFT-D approach has not been tested. The originally derived parameters have not been calibrated for host-guest interactions in nanoporous materials. The aim of this Master thesis is to test and recalibrate Van Der Waals interactions for nanoporous materials containing transition metals. With DFT-D methods one pursues a

reliable picture of adsorption and transport of guest molecules in the framework. The statistical physics of these phenomena is the basis for generic assessment procedures for the dispersion corrections. Both the development and the implementation of a quintessential quality measure of the DFT-D parameters are main deliverables of this thesis.

Promotoren: Prof. Dr. ir. V. Van Speybroeck - veronique.vanspeybroeck@ugent.be (09/264.65.58), Dr. ir. T. Verstraelen - toon.verstraelen@ugent.be (09/264.65.56) / **Begeleiding**: ir. L. Vanduyfhuys - louis.vanduyfhuys@ugent.be (09/264.65.60) / **http://molmod.ugent.be/student-corner**