

# Chemical systems and reactivity 2017-2018

## 1. Intermolecular Interactions

Coulombic interactions, polarisation effects and charge transfer

van der Waals interactions

$\pi - \pi$  interactions and  $\pi - \pi$  stacking

Hydrogen bonding

Halogen bonds

Hydrophobic effects

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The Theory of Intermolecular Forces, Anthony J. Stone, Clarendon Press, Oxford, 1996.

Supramolecular Chemistry Jonathan W. Steed, Jerry L. Atwood John-Wiley&Sons, 2000.

## 2. An Introduction to Density Functional Theory (DFT)

The expectation value of the energy is a functional of the wavefunction

The Hartree-Fock approximation

The density matrix and the electronic density

Expectation values and density matrix

Hartree-Fock and density matrix

DFT: basic principles

The Hohenberg-Kohn theorems

The Kohn-Sham method

The Kohn-Sham equations

The local density (LDA)

The generalized gradient approximation (GGA)

Recent developments of DFT and van der Waals interactions

The Jacob Ladder

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Density-Functional Theory of Atoms and Molecules. Robert G. Parr and Weitao Yang Oxford University Press, 1989

The ABC of DFT. Kieron Burke and friends Department of Chemistry, University of California, Irvine, CA 92697, 2007

<http://chem.ps.uci.edu/?kieron/dft/book/>

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### 3. Applications of Density Functional Theory (DFT)

$\pi$ -stacking of benzene monomers

Hydrogen-bonding interactions in complexes of benzene with polar species

van der Waals interactions and formation of free base phthalocyanine dimers

Complexation of calix[4]arenes with charged species

Endo- vs. exo-complexation in calix[4]arene-Ar<sub>2</sub> complexes

The structure of chlorophyll-c<sub>2</sub> in liquid methanol

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A Chemist's Guide to Density Functional Theory. Wolfram Koch, Max C. Holtausen Wiley-VCH, 2001

## 4. Fundamentals of Supramolecular Chemistry

Host-guest chemistry

Nature of Supramolecular Interactions

Porphyrins and tetrapyrrole macrocycles

Supramolecular features of Plant Photosynthesis

Crown ethers

Spherands

Cryptands

Calixarenes

Supramolecular Chemistry. Jonathan W. Steed, Jerry L. Atwood. John-Wiley&Sons, 2000.

Supramolecular Chemistry: Concepts and Perspectives. Jean-Marie Lehn. VCH, 1995.