Fluorinated biopolymers

Dispersion interactions in fluorinated biopolymers

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Kurzgefasst

- Fluorinated Biopolymers
- Dispersive Interactions
- Hydrophobic effect

Introduction

The structure and function of biopolymers are determined by the balance of different types of interactions: electrostatic, dispersion, and hydrophobic interactions. The latter are important in understanding the "hydrophobic effect" associated with aggregation of apolar solutes in aqueous environment. Dispersion interactions thus play a major role in the biopolymer structure and dynamics, leading to and stabilizing protein assemblies. Fluorination has been shown to modulate the properties of small molecules by altering the balance between electrostatic and dispersion interactions. Similar effects can be expected for peptides, proteins and other biopolymers. To explore the impact of fluorination on hydrated biopolymers, we will employ molecular simulations at atomic level detail, in comparison with Raman experiments provided by our collaboration partners. First principles simulations of fluorinated and non-fluorinated small molecules in gas phase and in solution will allow us to dissect the balance of electrostatic and dispersive interactions on an electronic structure level. These calculations will furthermore serve as reference data for the development of classical force field parameters. Using these parameters, classical molecular dynamics simulations on a larger scale will reveal the impact of fluorination on the dispersion interactions in biopolymers and their dependence on polymer *length*, *conformation,* and *structural flexibility.* These aspects which are important for proteins cannot be studied in the very small molecules typically used as analogues of amino acid side chains. However, direct dispersive interactions between hydrophobic groups in solution do depend on the distance of these groups and thus the shape and conformational dynamics of the polymer. Our simulations of selectively fluorinated biopolymers will probe whether dispersion interactions are the dominant contribution to hydrophobic attraction and may thus account for changes in protein structure and structural stability

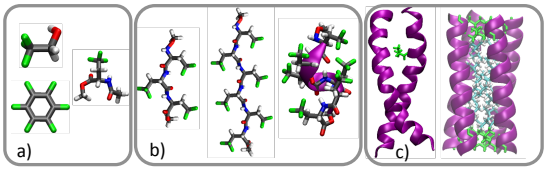

***Abbildung 1:** Example molecules/systems to be investigated: a) small molecules b) peptides c) coiled coils. green: fluorinated atoms (a,b) and amino acids (c).*

in fluorinated proteins. This understanding can ultimately be used to modify the balance of the different interactions and thereby control protein properties via specific fluor-substitution.

Keywords: Dispersion interaction, hydrophobic effect, fluorination, biopolymer aggregation, molecular simulations

Fluorinates amino acids, and fluorinated peptides will be investigated at a later stage of this project.

WWW

`https://www.uni-giessen.de/fbz/fb08/dispersion`

Weitere Informationen

Projektpartner

Markus Gerhards, Universtiät Kaiserslautern, Dor Ben-Amotz, Purdue University, Beate Koksch, FU Berlin

Förderung

DFG Schwerpunktprogramm SPP1807