Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Investigating of New Supramolecular Complexes



Project Manager
Prof. Dr. Hermann A. Wegner

Researchers
Daniel Kohrs

Principal Investigator
Prof. Dr. Hermann A. Wegner

Project Term
2019 - 2022

Clusters
Skylla Cluster Gießen, FUCHS-CSC Frankfurt

Software
GAUSSIAN

Institute
Institute of Organic Chemistry

University
Justus Liebig University Giessen

Introduction

Curved aromatic molecules are unique compounds as they combine special properties due to the delocalized π-system, with a 3D geometry. Thus, spherical aromatic compounds can interact via their convex surface with the concave hole of belt-shaped aromatic rings. With appropriate computational methods, these interactions can be predicted, supporting the design of suitable molecules for experiments. Therefore, high performance computation can help to reduce synthetic effort, as suitable candidates for supramolecular complexes can already be found in silico.

Methods

The Gaussian16 program package was used to identify target compounds and to evaluate potential interactions with selected macrocyclic aromatic hosts. Employing the M06-2X method, no additional corrections had to be employed, as this method already describes mid-range interactions properly. Regarding the size of the employed systems, Pople basis sets were applied, as these are computational comparable inexpensive. For the evaluation of the results, ChemCraft was used as an additional software.

Results

New supramolecular complexes were investigated within this project. Using DFT, the supramolecular entities were modelled, and possible structural arrangements and their energetic relation were predicted and compared. Also, different

substituents, capable of additional non-covalent interactions, were introduced to the backbone of the targeted nanorings. The competitive non-covalent interactions were investigated, as well as the possibility to tune them. The computational investigation of these properties will guide the synthetic design.

Outlook

Based on the interplay of experimental and computational data the optimal supramolecular assemblies will be established. These host-guest systems will be investigated in more detail to provide guidelines for the rational application of such weak interactions.

Publications

Y. Xu, M. von Delius, Angew. Chem. Int. Ed. 2020, 59, 559-573. https://doi.org/10.1002/anie.201906069

J. Rio, S. Beeck, G. Rotas, S. Ahles, D. Jacquemin, N. Tagmatarchis, C. Ewels, H. A. Wegner, Angew. Chem. Int. Ed. 2018, 57, 6930-6934. https://doi.org/10.1002/anie.201713197

T. Iwamoto, Y. Watanabe, T. Sadahiro, T. Haino, S. Yamago, Angew. Chem. Int. Ed. 2011, 50, 8342-8344. https://doi.org/10.1002/anie.201102302

Last Update: 2021-07-27 19:32