

Program

5th SPP 1807 “Summer School” Online

Control of London dispersion interactions in molecular chemistry

Thursday, March 4, 2021

1st Session: Spectroscopy I

Chair: Melanie Schnell

08:45-09:00	Peter R. Schreiner Opening remarks
09:00-09:20	Pablo Pinacho (DESY Hamburg) The effect of fluorine on the interaction contacts in large complexes: Diadamantyl-ether complexes with aromatic rings
09:20-09:40	Patrick Strebert (TU Kaiserslautern) Analysis of isolated molecular clusters in the gas phase
09:40-10:00	Felix Müller (U Bielefeld) Inter- and intramolecular interactions in bis(dimethylphosphino)methane
10:00-10:30	Break

2nd Session: Spectroscopy II

Chair: Martin Suhm

10:30-10:50	Charlotte Zimmermann (GAU Göttingen) Understanding structural preferences in ketone-solvent dispersion balances
10:50-11:10	Manuel Lange (GAU Göttingen) Aggregation of benzyl alcohol from a chiral and topological perspective
11:10-11:30	Robert Medel (GAU Göttingen) Chirality recognition and dispersion interaction in complexes of hydroxy compounds
11:30-11:50	Hannes Gottschalk (GAU Göttingen) The (fluorinated) acetophenone--methanol system: an intermolecular energy balance
11:50-13:00	Lunch break

3rd Session: Structure & Reactivity I

Chair: Ralf Ludwig

13:00-13:20	Marcel Strauss (JLU Giessen) London dispersion in alkane solvents
13:20-13:40	Anne Kunz (JLU Giessen) Intermolecular London dispersion interactions of azobenzene switches for tuning molecular solar thermal energy storage systems
13:40-14:00	Lars Rummel (JLU Giessen) Hydrohalogenation - A reaction to measure non-covalent interactions
14:00-14:30	Break

4th Session: Theory I

Chair: Giovanni Bistoni

14:30-14:50	Ephrath Solel (JLU Giessen) London Dispersion vs. steric hindrance
14:50-15:10	Eduardo Schiavo (MPI für Kohlenforschung, Mülheim a.d. Ruhr) Are heavy main group element - π interactions really “ π interactions”?
15:10-15:30	Ingolf Harden (MPI für Kohlenforschung, Mülheim a.d. Ruhr) Modeling complex catalytic reactions using high-level computational methods
15:30-16:00	Break

5th Session: Catalysis

Chair: Albrecht Berkessel

16:00-16:20	Torben Rogge (GAU Göttingen) Influence of dispersion on experimental and computational studies on catalyzed C-H activation
16:20-16:40	Wacharee Harnying (U Köln) NHC-catalyzed oxidative esterifications of aliphatic aldehydes/enals at low catalyst loadings
16:40-17:00	Stephanie Mayr (LMU München) Size-Induced Acylation of Aryl 1,2-Ethanediols
17:00-17:30	Break

6th Session: Spectroscopy IV

Chair: Ruth Gschwind

17:30-17:50	Matej Zabka (U Regensburg) The late and the weak: Intermediates and interactions in catalysis by combined NMR and computational approach
17:50-18:10	Johannes Gramüller (U Regensburg) Accessing the role of dispersion Interactions in Brønsted acid catalysis by NMR spectroscopy
18:10-18:30	Adélaïde Savoy (ETH Zürich) Intramolecular bent hydrogen bonds in bipyridines - geometry and chemical shifts
18:30-19:00	Break

1st Invited Talk: Catalysis

Chair: Jan Paradies

19:00-20:00	Henrik Zipse (LMU München) Size-induced selectivity in esterification reactions
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7th Session: Structure & Reactivity II

Chair: Peter R. Schreiner

09:00-09:20	Henrik König (JLU Giessen) Dispersion guided aggregation of organic dye molecules
09:20-09:40	Finn Wilming (JLU Giessen) Quantifying London dispersion with 2,2'-substituted 9,9'-bifluorenylidenes
09:40-10:00	Marvin Domanski (JLU Giessen) Influence of dispersion energy donors on the folding of N',N'-diphenylthioureas
10:00-10:30	Break

8th Session: *Chair: Spectroscopy III*

Peter Chen

10:30-10:50	Vladimir Gorbachev (ETH Zürich) Determination of spectroscopically-structural connections in the pyridinium series to probe London dispersion forces
10:50-11:10	Alexandra Tsybizova (ETH Zürich) Modulating bond strengths in large molecules. Stretching the limits.
11:10-11:30	Johannes Fischer (U Regensburg) The high resolution electronic spectra of large molecules and v. d. W.-clusters. I: Helium nanodroplet studies
11:30-11:50	Florian Schlaghauser (U Regensburg) The high-resolution electronic spectra of large molecules and v.d.W.-clusters: II Gas phase studies
11:50-13:00	Lunch break

9th Session: Theory II

Chair: Ana Vila Verde

13:00-13:20	Philipp Dullinger (U Regensburg) MD simulations regarding the solvation and structuring of ions in a fluorinated solvent
13:20-13:40	Federica Ferraro (FAU Erlangen) Study of the influence of intramolecular versus solute-solvent interactions on fluorinated and non-fluorinated amino acids
13:40-14:00	Juana Vázquez Quesada (KIT) A litmus test for the description of dispersion interaction
14:00-14:30	Break

10th Session: Structure & Reactivity III

Chair: Frank Biedermann

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| 14:30-14:50 | Alexander Gehlhaar (U Duisburg-Essen)
Inter- and intramolecular interactions in homoleptic naphthylpnictanes |
| 14:50-15:10 | Laura Grimm (KIT)
Systematic investigations of cucurbit[n]uril-guest complex formation by ITC and fluorescence titration experiments |
| 15:10-15:30 | Sebastian Scholz (TU Chemnitz)
Bismuth as a dispersion energy donor in molecular chemistry |
| 15:30-16:00 | Break |

11th Session: Structure & Reactivity IV

Chair: Guido Clever

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| 16:00-16:20 | Andre Platzek (TU Dortmund)
Substrate and product binding inside a singlet oxygen photosensitizing nano cage |
| 16:20-16:40 | Christoph Drechsler (TU Dortmund)
Investigation and simulation of supramolecular coordination cages with ion mobility spectrometry |
| 16:40-17:00 | Stanislav Kondratev (U Rostock)
Stabilizing power of dispersion forces in aromatic compounds |
| 17:00-17:30 | Break |

12th Session: Structure & Reactivity V

Chair: Sergey Verevkin

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| 17:30-17:50 | Zheng-Wang Qu (RFWU Bonn)
Transition-metal-free Fischer-Tropsch chemistry |
| 17:50-18:10 | Hui Zhu (RFWU Bonn)
Dimethyl sulfoxide (DMSO) catalyzed aromatic chlorination |
| 18:10-18:30 | Benedikt Sieland (U Paderborn)
Stabilization of frustrated Lewis pairs by London dispersion interactions |
| 18:30-19:00 | Break |

2nd Invited Talk: Theory

Chair: Bretislav Friedrich

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| 19:00-20:00 | Denis Usvyat (HU Berlin)
Nailing down van der Waals dispersion in periodic systems: A quantum chemical route |
| 20:00-20:15 | Peter R. Schreiner
Closing remarks |