

Topological Approaches to Intermolecular Interactions

Timetable

	Tuesday 25 th	Wednesday 26 th	Thursday 27 th	Friday 28 th
	TRAINING	WORKSHOP		
9:00-9:30	ELF/NCI/MPDs	Opening	Coffee	Coffee
9:30-10:00		Frank de Proft	Manuel Yáñez	Weitao Yang
10:00-10:30		BREAK	BREAK	BREAK
10:30-11:00		Piotr da Silva	Marc García-Borràs	Vincent Tognetti
11:00-11:30		Gabriele Saleh	Mercedes Alonso	Verónica Postils
11:30-12:00		Eduard Matito	Mónica Calatayud	Alberto Otero-de-la-Roza
12:00-12:30		LUNCH (not provided)	LUNCH	LUNCH
12:30-14:30	LUNCH (not provided)	LUNCH	LUNCH	
14:30-15:00	NCI exptal. Densities	Ángel Martín Pendás	VISITS	Slawomir J. Grabowski
15:00-15:30	NCI solids	BREAK		BREAK
15:30-16:00	MPDs	Silvia Simon	Paul Popelier	Benoit de Courcy
16:00-16:30		Ferràn Feixas		Kasper Mackeprang
16:30-17:00	aNCI	Piotr Kasprzycki	Hélène Gerard	Christine Lepetit
17:00-17:30		Kati Finzel	Robin Chaudret	Odile Eisenstein
17:30-18:00	Discussion	Dylan Jayatilaka	Arturo Espinosa	Discussion
18:00-18:30		Discussion		Closing
18:30-19:00		Poster session		
19:00-19:30				
19:30-20:00				
20:00-20:30			DINNER	
who knows				

Detailed Program

Wednesday 26th

Chairperson: Jean Philip Piquemal

9:30-10:30 Frank de Proft

Combined use of DFT based Reactivity Indices and the Non-covalent Index in the Study of Intermolecular Interactions

10:30-11:00 **BREAK**

11:00-11:30 Piotr de Silva

[Probing Aromaticity and Non-Covalent Interactions with Single Exponential Decay Detector \(SEDD\)](#)

11:30-12:00 Gabriele Saleh

[Exploring non-covalent interactions in molecular crystals through the analysis of their experimental electron density distribution](#)

12:00-12:30 Eduard Matito

[Multicenter Bond Index: a versatile tool to characterize electron delocalization and aromaticity](#)

12:30-14:30 **LUNCH**

Chairperson: Eduard Matito

14:30-15:30 Ángel Martín Pendás

[Decay rate of delocalization indices: towards a real space image of the insulating or metallic character of a material](#)

15:30-16:00 **BREAK**

16:00-16:30 Sílvia Simon

[Delocalization Indices for Non-Covalent Interaction](#)

16:30-17:00 Ferran Feixas

[The role of cis-prenyl diphosphate synthases in bacterial cell-wall biosynthesis: non-covalent interactions and its implications for drug discovery](#)

17:00-17:30 Piotr Kasprzycki

[The correlation between the proton transfer time and electron density in the inner cavity of porphycenes](#)

17:30-18:00 Kati Finzel

[Indicators based on electron density inhomogeneity](#)

18:00-18:30 Dylan Jayatilaka

[Some thoughts about efficient implementation of accurate intermolecular interaction energies](#)

18:00-18:30 **DISCUSSION**

Discussion leader: Andreas Savin

18:30-20:00 **POSTER SESSION**

Thursday 27th

Chairperson: Peter Reinhardt

9:30-10:30 Manuel Yáñez

[Playing around with Beryllium Bonds](#)

10:30-11:00 **BREAK**

11:00-11:30 Marc Garcia-Borràs

[Intermolecular Dispersion Interaction Effects on the Diels-Alder Endohedral Metallofullerene Monoadduct stabilities. The Cp/Cp*-La@C_{2v}-C₈₂ example.](#)

11:30-12:00 Mercedes Alonso

[Fine-tuning of the conformation of expanded porphyrins using conceptual DFT descriptors and non-covalent index](#)

12:00-12:30 Mónica Calatayud

[Reactivity indices and bonding in V₂O₅ based materials](#)

12:30-14:30 **LUNCH**

14:30-16:00 VISITS

Chairperson: Odile Eisenstein

16:00-17:00 Paul Popelier

Quantum Chemical Topology: on Bonds and Force Fields

17:00-17:30 Hélène Gerard

Interactions within heterobimetallic complexes

17:30-18:00 Robin Chaudret

Non covalent interaction within reactive and dynamic systems : a presentation of ELF/NCI and aNCI

18:00-18:30 Arturo Espinosa

Intra- and intermolecular NCIs balance in biscarbazole-trisurea (BC3U) receptors and their pyrophosphate complexes

20:00 **DINNER**

Friday 28th

Chairperson: Robin Chaudret

9:30-10:30 Weitao Yang

Non-Covalent Interaction Analysis in Fluctuating Environments and Exchange-Correlation Energies from Response Properties

10:30-11:00 **BREAK**

11:00-11:30 Vincent Tognetti

QTAIM/DFT descriptors for the description of “weak” interactions

11:30-12:00 Verònica Postils

[Characterization and Identification of Electrines](#)

12:00-12:30 Alberto Otero-de-la-Roza

[Exchange and correlation effects on non-covalent interactions](#)

12:30-14:30 **LUNCH**

Chairperson: Henry Chermette

14:30-15:30 Slawomir J. Grabowski

[Non-covalent interactions: characteristics and mechanisms of formation - the topological approach](#)

15:30-16:00 **BREAK**

16:00-16:30 Benoit de Courcy

[TBA](#)

16:30-17:00 Kasper Mackeprang

[Weak intramolecular OH \$\cdots\$ \$\pi\$ hydrogen bonding in methallyl and allyl carbinol](#)

17:00-17:30 Christine Lepetit

[Theoretical studies of the metal-phenylene interaction in a P\(CH\)P pincer rhodium\(I\) complex](#)

17:30-18:00 Odile Eisenstein

[Analysis of weak interactions for asymmetric synthesis: the case of the selective hydrogenation of artemisinic acid by diazene](#)

18:00-18:30 **DISCUSSION**

Discussion leader: Erin Johnson

18:30-17:00 CLOSING