

# Timetable

	Tuesday 25 <sup>th</sup>	Wednesday 26 <sup>th</sup>	Thursday 27 <sup>th</sup>	Friday 28 <sup>th</sup>	
	<b>TRAINING</b>		<b>WORKSHOP</b>		
9:00-9:30	ELF/NCI	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		Alberto Otero-de-la-Roza	Marc García-Borràs	Vincent Tognetti	
11:00-11:30		Gabriele Saleh	Mercedes Alonso	Verónica Postils	
11:30-12:00		Eduard Matito	Mónica Calatayud	Piotr de Silva	
12:00-12:30	FREE LUNCH	LUNCH	LUNCH	LUNCH	
12:30-14:30					
14:30-15:00	NCI exptal. Densities	Ángel Martín Pendás	VISITS	Slawomir J. Grabowski	
15:00-15:30				BREAK	
15:30-16:00	NCI solids	BREAK	Paul Popelier	Kasper Mackeprang	
16:00-16:30		Silvia Simon		Christine Lepetit	
16:30-17:00	MPDs	Ferràn Feixas		Odile Eisenstein	
17:00-17:30		Piotr Kasprzycki	Hélène Gerard		
17:30-18:00	aNCI	Discussion	Robin Chaudret	Discussion	
18:00-18:30			Arturo Espinosa	Closing	
18:30-19:00		Poster session			
19:00-19:30					
19:30-20:00					
20:00			DINNER		
who knows					

## Detailed Program

### Wednesday 26<sup>th</sup>

Chairperson:

#### 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 Alberto Otero-de-la-Roza

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

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:

**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 **DISCUSSION**

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

**Thursday 27<sup>th</sup>**

*Chairperson:*

**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<sub>2v</sub>-C<sub>82</sub> 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

[TBC](#)

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

14:30-16:00 VISITS

*Chairperson:*

**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 28<sup>th</sup>**

*Chairperson:*

**9:30-10:30 Weitao Yang**

[TBA](#)

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 Electrides](#)

12:00-12:30 Piotr de Silva

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

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

*Chairperson:*

**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 Kasper Mackeprang

*Weak intramolecular OH $\cdots$  $\pi$  hydrogen bonding in methallyl and allyl carbinol*

16:30-17:00 Christine Lepetit

*Theoretical studies of the metal-phenylene interaction in a P(CH)P pincer rhodium(I) complex*

**17:00-17:30 Odile Eisenstein**

*TBA*

17:30-18:00 **DISCUSSION**

18:00-18:30 **CLOSING**