Scientific program

Monday, May 13

8:15-8:45 ***Opening***

Philippe RAIMBAULT (President of Université de Toulouse)

Michel CAFFAREL (Toulouse)

Chair: Zhigang SHUAI (Beijing)

8:45-9:45 ***Session 1: Catalysis and material design I***

8:45-9:05 **Jinlong YANG** (Hefei)

Two-dimensional materials design for photocatalytic water splitting from a theoretical perspective.

9:05-9:25 **Marie-Liesse DOUBLET** (Montpellier)

Chemical bonding approaches to energy materials

9:25-9:45 Discussion

9:45-10:45 ***Session 2: Catalysis and material design II***

9:45-10:05 **Xin XU** (Fudan)

Towards accurate and efficient microkinetic modelling in heterogeneous catalysis.

10:05-10:25 **Aude SIMON** (Toulouse)

PAHs adsorbed on interstellar ice: structures, energetics and IR spectra from a multi-method approach.

10:25-10:45 Discussion

10:45-11:00 **Coffee break**

Chair: ***Michel CAFFAREL*** (Toulouse)

11:00-12:00 ***Session 3: Catalysis and material design III***

11:00-11:20 **Zhipan LIU** (Fudan)

Machine Learning for resolving the global potential energy surface and predicting catalysis.

11:20-11:40 **Jean-Sebastien FILHOL** (Montpellier)

Interface Electrochemistry.

11:40-12:00 Discussion

12:15-2:30 **Lunch** at restaurant “Chez Navarre” 49 grande rue Nazareth Toulouse

Chair: ***Wenjian LIU*** (Shandong)

2:30-3:30 ***Session 4: Relativistic quantum chemistry***

2:30-2:50 **Nicolas GALLAND** (Nantes)

A relativistic perspective on halogen bonding.

2:50-3:10 **Jun LI** (Tsinghua)

Relativity breaks periodicity of chemical bonding in heavy-element compounds.

3:10-3:30 Discussion

3:30-4:30 ***Session 5: Valence bond***

3:30-3:50 **Peter REINHARDT** (Paris)

Dispersion interactions in a VB context.

3:50-4:10 **Peifeng SU** (Xiamen)

A valence bond based energy decomposition analysis scheme for non-covalent interaction and chemical bond.

4:10-4:30 Discussion

4:30-5:00 **Coffee break**

Chair: ***Wenjian LIU*** (Shandong)

5:00-6:00 ***Session 6: Solid/Surface***

5:00-5:20 **Hasar GUESMI** (Montpellier)

Reshaping dynamics and atomic ordering changes in metallic and alloy nanoparticles under reactive gas: theoretical multiscale methods.

5:20-5:40 **Jinlan WANG** (Nanjing)

Accelerated discovery of stable lead-free photovoltaic perovskites via machine learning.

5:40-6:00 Discussion

7:30 **Dinner** at restaurant “Au Gascon” 9 Rue des Jacobins Toulouse

Tuesday, May 14

	Chair: ***Nicolas FERRE*** (Marseille)
8:30-9:30	***Session 7: Proteins I***
8:30_8:50	**Yundong WU** (Shenzen)
	Force fields for the simulations of intrinsically disordered proteins.
8:50-9:10	**Thomas SIMONSON** (Palaiseau)
	Engineering proteins with computer simulations: the example of PDZ: peptide binding.
9:10-9:30	Discussion
9:30-10:30	***Session 8: Proteins II***
9:30-9:50	**Guohui LI** (Dalian)
	Multiscale modeling of dynamics and mechanism of functions of biomolecules.
9:50-10:10	**Matthieu MONTES** (Paris)
	Enhancing the user-interaction with a molecular system using Udock.
10:10-10:30	Discussion
10:30-11:00	**Coffee break**
	Chair: ***Stefano EVANGELISTI*** (Toulouse)
11:00-12:00	***Session 9: Non-diabatic dynamics***
11:00-11:20	**Zhenggang LAN** (Guangzhou)
	Machine learning in nonadiabatic dynamics.
11:20-11:40	**Patrick CASSAM-CHENAI** (Nice)
	Electronic basis functions for smeared atomic densities.
11:40-12:00	Discussion
12:15-2:30	**Lunch** at restaurant "Chez Navarre" 49 grande rue Nazareth Toulouse
	Chair: Weihai FANG (Beijing)
2:30-3:30	***Session 10: QM/MM I***
2:30-2:50	**Fabris KOSSOSKI** (Aix-Marseille)
	Direct dynamics simulation of electron-induced dissociation of chloroethane.
2:50-3:10	**Lin SHEN** (Beijing)
	Development of multiscale QM/MM method combined with resolution-adapted and neural network models.
3:10-3:30	Discussion

3:30-4:30 ***Session 11: QM/MM II***

3:30-3:50 **Isabelle NAVIZET** (Marne la Vallée)

Importance of the modelling of the surrounding environment: example of absorption and emission spectra of oxyluciferin analogues.

3:50-4:10 **Jing MA** (Nanjing)

A data-driven accelerated sampling method for simulations of conformational changes in condensed phase.

4:10-4:30 Discussion

4:30-5:00 **Coffee break**

Chair: Hélène BOLVIN (Toulouse)

5:00-6:00 ***Session 12: Organometallics***

5:00-5:20 **Karine COSTUAS** (Rennes)

Quantum chemical studies of metal-containing compounds for molecular optoelectronics.

5:20-5:40 **Zhenyang LIN** (Hong Kong)

Unravelling chemical interactions with principal interacting orbital (PIO) analysis.

5:40-6:00 Discussion

7:30 **Workshop dinner** at Restaurant "Les Arcades" Place du Capitole Toulouse

Wednesday, May 15

	Chair: Jean-Paul MALRIEU (Toulouse)
8:30-9:30	***Session 13: Post-Hartree Fock methods***
8:30_8:50	**Shuhua LI** (Nanjing)
	"Cluster-in-molecule" local correlation approach for large molecules and periodic systems.
8:50-9:10	**Emmanuel GINER** (Paris)
	A density-based basis-set correction for wave function theory.
9:10-9:30	Discussion
9:30-10:30	***Session 14: Spectroscopy***
9:30-9:50	**Zhigang SHUAI** (Beijing)
	Numerical solutions to optical spectroscopy for molecular aggregates using TD-DMRG: comparison for time domain and frequcency domain algorithms.
9:50-10:10	**Valérie BRENNER** (Gif sur Yvette)
	Conformational landscape and electronic dynamics of model proteins chains.
10:10-10:30	Discussion
10:30-11:00	**Coffee break**
	Chair: Gilberte CHAMBAUD (Marne la Vallée)
11:00-12:00	***Session 15: Dynamics***
11:00-11:20	**Donghui ZHANG** (Dalian)
	Time-dependent wave packet studies of chemical reactions.
11:20-11:40	**Roberto MARQUARDT** (Strasbourg)
	The quantum dynamics of resonances: An exact, time reversible solution.
11:40-12:00	Discussion
12:00-12:10	**Isabelle NAVIZET** (Marne la Vallée)
	Closing remarks
12:20-2:30	**Lunch** at restaurant "Chez Navarre" 49 grande rue Nazareth Toulouse