GDR EMIE - GRANDS INSTRUMENTS POUR LA PHYSICO-CHIMIE MOLÉCULAIRE

Asnelles sur mer (Calvados), France, October 11-14, 2021

Monday 11th October 2021	
	DAY 1
15:00-15:45	Registration
	Session 1 – Ions across the axis, *Chair: Patrick Rousseau (UNICAEN)*
15:45-16:20	*Ion-collision induced dynamics of complex molecular systems in the gas phase* **Alicja Domaracka,** Normandie Université, CIMAP, Caen, France
16:20-16:55	*Swift heavy ions and complex organic molecules in the solid phase for astrophysics* **Philippe Boduch,** Normandie Université, CIMAP, Caen, France
16:55-17:30	*Slow relaxation processes of cationic PAHs stored in electrostatic storage rings, DESIREE and Mini-Ring* **Jérôme Bernard,** Université Claude Bernard, ILM, Lyon, France
17:30-18:00	***Coffee break***
	Session 2 – Instrumental developments, *Chair: Aleksandar Milosavljevic (SOLEIL)*
18:00-18:20	*DESIREE: The Cryogenic Electrostatic Storage Ring* **Suvasthika Indrajith,** Stockholm University, Stockholm, Sweden
18:20-18:40	*Development of an electrostatic ion beam trap and its applications* **Raj Singh,** CIMAP, GANIL, Caen, France
18:40-19:00	*New Spectroscopic Methods for THz Synchrotron Beamlines* **Thomas S Hearne,** Université Paris-Saclay, ISMO, Orsay, France
19:00-19:20	*Performance and first results of a versatile home-built tandem mass spectrometer dedicated for experiments at advanced light sources* **Juliette Leroux,** Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany
	Dinner

Tuesday 12th October 2021	
	DAY 2
08:30-08:50	Registration
08:50-09:00	Opening and Introduction **Pierre Carcabal,** ISMO
	Grands instruments and theory, *Chair: Pierre Carcabal (ISMO)*
09:00-09:45	*Les TGIR à l'Institut de Physique du CNRS* **Sylvain Ravy,** CNRS, INP, France
09:45-10:20	*Equivocal identification of gas phase medium sized molecular species in mixture by high accuracy single photon ionization and ab initio computations* **Majdi Hochlaf,** Université Gustave Eiffel, COSYS/LISIS, Marne-la-Vallée, France
10:20-10:50	***Coffee break***
	Session 3 – Excited states, *Chair: Laurent Nahon (SOLEIL)*
10:50-11:25	*X-ray induced ultrafast dynamics in excited molecules* **Oksana Travnikova,** Sorbonne Université, LCPMR, Paris, France
11:25-11:45	*State-selected ion-molecule reactions with VUV synchrotron radiation of interest for depollution plasma development* **Roland Thissen,** Université Paris-Saclay, ICP, Orsay, France
11:45-12:05	*Photoelectron spectroscopy and circular dichroism of chiral oxirane radicals* **Gustavo Garcia,** Synchrotron SOLEIL, Saint Aubin, France
12:05-12:25	*Cage-opening dynamics of adamantane* **Sylvain Maclot,** University of Gothenburg, Gothenburg, Sweden
12:30-15:30	***Lunch break***

	Session 4 – Astrophysics and atmosphere, *Chair: Olivier Pirali (ISMO)*
15:30-16:05	*Enabling interstellar detections using synchrotron-based far-infrared spectroscopy* **Marie-Aline Martin-Drumel,** Université Paris-Saclay, ISMO, Orsay, France
16:05-16:40	*Vacuum-UV and soft X-ray induced photodesorption from molecular ices* **Mathieu Bertin,** Sorbonne Université, LERMA, Paris, France
16:40-17:15	*High-resolution far-infrared spectroscopy of spherical-top molecules using synchrotron radiation* **Vincent Boudon,** Université de Bourgogne, ICB, Dijon, France
17:15-17:35	*Competing energy dissipation pathways at the gas-grain interface: a study of astrophysically-relevant ices* **Jennifer Noble,** Aix-Marseille Université, PIIM, Marseille, France
17:35-18:00	***Coffee break***
	Conférence grand public, *Chair: Alicja Domaracka (CIMAP)*
18:00-19:00	*De Curie au GANIL* **David Boilley,** Normandie Université, GANIL, Caen, France
	Free time and Dinner

Wednesday 13th October 2021	
	DAY 3
	Session 5 – Free electron lasers, *Chair: Marc Simon (LCPMR)*
09:00-09:35	*Femtosecond molecular dynamics at free-electron laser sources* **Maria Novella Piancastelli,** Uppsala Universitet, Sweden and Sorbonne Université, LCPMR, Paris, France
09:35-10:10	*Free Electron Laser and IRMPD Spectroscopy: a perfect synergy to unravel the structure and reactivity of biomolecules in the gas phase* **Debora Scuderi,** Université Paris Saclay, ICP, Orsay, France
10:10-10:30	*Application of near edge X-ray absorption mass spectrometry for the study of bio-relevant molecules in the gas phase* **Lucas Schwob,** Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany
10:30-11:00	***Coffee break***
	Session 6 – Biomolecules, *Chair: Debora Scuderi (ICP)*
11:00-11:35	*Activation and spectroscopy of mass and charge selected ions stored in a linear ion trap* **Alexandre Giuliani,** INRA and Synchrotron SOLEIL, Saint Aubin, France
11:35-11:55	*Photo and Auger electron spectroscopies of phthalocyanines in the gas phase* **Gildas Goldsztejn,** Université Paris-Saclay, ISMO, Orsay, France
11:55-12:15	*Ion-collision dynamics of complex molecular systems in the gas phase* **Min Liu,** ENSICAEN, UNICAEN, CEA, CNRS, CIMAP, Caen, France
12:15-12:35	*Photoelectron circular dichroism as a probe for conformational isomerism in 1-indanol* **Jennifer Dupont,** Université Paris-Saclay, ISMO, Orsay, France
12:35-15:00	***Lunch break***
15:00-17:30	***Free time and Outdoor activities***
	Round table: "Grand Instruments pour la physico-chimie moléculaire", *Chair: Roland Thissen (ICP)*

17:30-19:30	1. *Future Plans and Major Evolutions:*
	   a. *CLIO (D. Scuderi)*
	   b. *SOLEIL (L. Nahon)*
	   c. *GANIL (to be announced)*
	2. *Organizations and Representation of Users:*
	   a. *GDR X-FEL (M. Simon)*
	   b. *GDR EMIE (P. Carcabal)*
	   c. *Users Organizations: Orgues, AFURS, ESUO*
	3. *Users Access*
	4. *Young Researchers and Trainees*

	Dinner

Thursday 14th October 2021	
DAY 4	
	Session 7 – Aggregates and environmental effects - 1, *Chair: Simon Aude (LCPQ - IRSAMC)*
09:00-09:35	*Surface chemistry of gold nanoparticles produced by laser ablation and perspectives as photosensitizers* **Anna Lévy,** Sorbonne Université, INSP, Paris, France
09:35-10:10	*Photoelectron angular distributions of chiral aerosol particles: Condensation effects on chiral asymmetries* **Sebastian Hartweg,** Synchrotron SOLEIL, Saint Aubin, France
10:10-10:30	*Investigation of ligand electronic effects on iron cyclopentadienyl complexes using photoelectron spectroscopy* **Lyna Bourehil,** Synchrotron SOLEIL, Saint Aubin, France
10:30-11:00	***Coffee break***
	Session 8 – Aggregates and environmental effects - 2, *Chair: Pierre Carcabal (ISMO)*
11:00-11:35	*Overview of neutron spectroscopic techniques and insight into the microscopic properties of water confined in nanopores* **Marie Plazanet,** INRA and Synchrotron SOLEIL, Saint Aubin, France
11:35-12:10	*Jet-cooled far-infrared spectroscopy of molecules on the AILES beamline of SOLEIL* **Robert Georges,** Université Rennes 1, IPR, Rennes, France
12:10-12:30	*On the structure and electronic spectra of excited neutral argon rare gas clusters using Hole Particle Pseudopotential method* **Mukul Dhiman,** ENSICAEN, UNICAEN, CEA, CNRS, CIMAP, Caen, France
12:30-12:50	*Toward a better description of proteins electronic structure in a solvated state using electron spectroscopy* **Lucie Huart,** NIMBE, IRAMIS, CEA and Synchrotron SOLEIL, Saint Aubin, France
13:00-15:00	***Lunch***
	Departure

COLOR LEGEND

Yellow – Selected oral contributions: 20 min (5 min for questions and discussion)
Green – Invited lectures: 35 min (5-10 min for questions and discussion)
Blue – Plenary lecture: 45 min (35-40 min + 5-10 min); Conférence grand public: 60 min; Round table: 120 min

INSTITUTIONS' ACRONYMS (in the order of appearance)

UNICAEN - Université de Caen Normandie (Caen)
CIMAP - Centre de recherche sur les Ions, les Matériaux et la Photonique (Caen)
ILM – Institut Lumière Matière (Lyon)
GANIL – Grand Accélérateur National d'Ions Lourds (Caen)
ISMO – Institut des Sciences Moléculaires d'Orsay (Orsay)
TGIR – Les très grandes infrastructures de recherche (France)
CNRS – Centre National de la Recherche Scientifique (France)
INP – Institut de Physique (France)
COSYS – Composantes et Systèmes (Univ. Gustave Eiffel, Champs-sur-Marne)
LISIS – Instrumentation, Simulation et Informatique Scientifique (Univ. Gustave Eiffel, Champs-sur-Marne)
SOLEIL – Source Optimisée de Lumière d'Energie Intermédiaire du LURE (France)
(LURE - Laboratoire d'Utilisation du Rayonnement Électromagnétique)
LCPMR – Le Laboratoire de Chimie Physique-Matière et Rayonnement (Paris)
ICP - Institut de Chimie Physique (Orsay)
LERMA – Laboratoire d'Etudes du Rayonnement et de la Matière en Astrophysique et Atmosphères (Paris)
ICB – Laboratoire Interdisciplinaire Carnot de Bourgogne (Dijon)
PIIM – Physique des Interactions Ioniques et Moléculaires (Marseille)
INRA – Institut National de la Recherche Agronomique (France)
IPR – Institut de physique de Rennes (Rennes)
ENSICAEN – National Graduate School of Engineering and Research Center (Caen)
CEA – Commissariat à l'énergie atomique et aux énergies alternatives (France)
NIMBE – Nanosciences et Innovation pour les Matériaux, la Biomédecine et l'Énergie (Saclay)
IRAMIS – L'Institut Rayonnement-Matière de Saclay (Saclay)

GDR – Groupement de recherche (CNRS)
EMIE – Edifices Moléculaires Isolés et Environnés (GDR CNRS)
X-FEL – X-ray Free Electron Laser