The 9th NIMS-UnivRen-CNRS-SG Workshop

Materials and Sustainable Development: Issues and Challenges of the 21st Century

Date: June 2-4th, 2024

Venue: PNRB, Campus de Beaulieu, Université de Rennes, France

Organized by

National Institute for Materials Sciences

CNRS

Saint-Gobain

The University of Rennes

Organizing committee:

Dr. J.-F. HALET (Co-chair, ISCR, CNRS)
Dr. F. TESSIER (Co-chair, ISCR, CNRS)

Dr. D. BERTHEBAUD (IMN, CNRS)
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Financial support

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PNRB Auditorium, Campus de Beaulieu, 263 Av. Général Leclerc, Rennes Univ.

- Free registration on https://ws9nimsrennes.sciencesconf.org/?lang=en

- All coffee breaks, lunches and dinners are provided only upon invitation

Sunday, JUNE 2 2024		
18:00-19:00 Registration		
18:30-20:30 Welcome Party at MERCURE Hotel Centre Gare		
Monday, JUNE 3 2024		
08:30-09:00	Registration	
Chairs: Franck TESSIER and Jean-François HALET		
09:00-10:15	**Welcome by Marc FOURMIGUE**	
Time	Speaker	Title
Session I: Materials by Design		
09:15-09:55	**Keynote Talk**	
	Gilles FRAPPER (IC2MP-Poitiers Univ.)	EMERGENCE OF POLYNITROGEN NETWORKS IN LEAD-NITROGEN PbNx PHASES UNDER PRESSURE
09:55-10:25	**Coffee break and Poster session**	
Chairs: Jean-Marc JOUBERT and David BERTHEBAUD		
10:25-10:40	**Guillaume LAMBARD** (NIMS-LINK)	ACTIVE LEARNING APPLIED TO MATERIALS SCIENCE
10:40-10:55	**Régis GAUTIER** (ISCR-ENSCR)	THERMOELECTRIC MATERIALS: A LONG-TERM AND FRUITFUL COLLABORATION BETWEEN EXPERIMENTALISTS AND THEORETICIANS IN THE FRAMEWORK OF LINK
10:55-11:10	**Jia ZHU** (SGRS) (by zoom)	MATERIALS INFORMATICS: UTILIZING AI TO ASSIST PRODUCT FORMULATION DESIGN
11:10-11:25	**Jean-Claude CRIVELLO** (LINK-CNRS)	DESIGNING HYDRIDES FOR HYDROGEN STORAGE USING MACHINE LEARNING
Chairs: Jean-Claude CRIVELLO and Guillaume LAMBARD		
11:25-11-40	**Loïc LE TIRAN** (SGRP)	MATERIAL INFORMATICS FOR SG MATERIALS
11:40-11:55	**Sylvain LETONQUESSE** (CRISMAT-CNRS)	FAST OPTIMIZATION OF MATERIAL SYNTHESIS VIA BAYESIAN OPTIMIZATION: A CASE STUDY ON MAGNETOCALORIC $Mn_{5-X}Fe_XSi_3$
11:55-12:10	**Jean-Marc JOUBERT** (ICMPE-CNRS)	THE CALPHAD METHOD FOR MATERIALS DESIGN

12:10-14:00	**Lunch buffet and Poster session**	
	Session II: Materials for Energy and Environment	
	Chairs: Hiroyo SEGAWA and Stéphane CORDIER	
14:00-14:15	**Naoki OHASHI** (NIMS-LINK)	SOME INSIGHTS ON Mo_6 CLUSTER COMPLEX AND ITS RELATED COMPOUNDS FROM RECENT INVESTIGATION
14:15-14:30	**Adèle RENAUD** (ISCR-Rennes Univ.)	OCTAEDRAL METAL CLUSTER-BASED BUILDING BLOCKS: TOWARDS THE ENGINEERING OF NEW AMBIPOLAR PHOTOELECTRODES FOR SOLAR ENERGY CONVERSION
14:30-14:45	**Tetsuo UCHIKOSHI** (NIMS-LINK)	LIGHT AND HUMIDITY SENSING BY Mo_6 CLUSTER FILM FABRICATED BY ELECTROPHORETIC DEPOSITION
14:45-15:00	**Clément LEBASTARD** (LINK-CNRS)	ELABORATION OF HYBRID THIN FILM BY ECTROPHORETIC DEPOSITION: FROM NANOPARTICLES TO DEVICES
15:00-15:15	**Florent PAWULA** (IMN-Nantes Univ.)	HYBRID LEAD HALIDE PEROVSKITE SINGLE CRYSTAL: STRUCTURAL, OPTICAL, AND THERMAL PROPERTIES
15:15-15:45	**Coffee Break and poster session**	
	Chairs: Adèle RENAUD and Philippe THOMAS	
15:45-16:00	**Adrian DAVID** (CRISMAT-UNICAEN)	STRATEGIES FOR ACHIEVING A LARGE OPTICAL TRANSPARENCY WINDOW IN CORRELATED TRANSPARENT CONDUCTORS
16:00-16:15	**Daiki UMEYAMA** (NIMS)	MOLECULAR CONTROL OF THE STEREOCHEMICAL ACTIVITY OF Pb(II) LONE PAIR FOR DESIGNING ORGANIC-INORGANIC VALENCE BAND DISPERSIONS
16:15-16:30	**Sadaki SAMITSU** (NIMS)	FABRICATION AND CHARCTERIZATION OF POROUS POLYMERS
16:30-16:45	**Corinne LAGROST** (ISCR-CNRS)	HYBRID CALIX[4]ARENE-PLATINUM NANOPARTICLES FOR RECONCILING ORR AND MOR ELECTROCATALYSES
16:45-17:00	**Yoshiyuki SUGAHARA** (Waseda Univ.)	USE OF AN IRON-DOPED COBALT-MOLYBDENUM-DITHIOOXAMIDE COMPLEX FOR ELECTROCATALYTIC WATER OXIDATION
17:00-17:15	**Thierry GLORIANT** (ISCR-INSA)	OUTSTANDING STRAIN-HARDENING OF A NEW METASTABLE BETA-TITANIUM ALLOY ELABORATED BY IN SITU ADDITIVE MANUFACTURING L-PBF PROCESS
17:15-17:30	**Noriko SAITO** (NIMS-LINK)	GAS SENSOR APPLICATIONS OF SEMICONDUCTIVE NANOPARTICLES
17:30-17:45	**Marielle THIBAULT** (ZirPro)	CERAMIC POWDERS FOR HYDROGEN PRODUCTION THROUGH ALKALINE ELECTROLYSIS
17:45-18:00	**Hiroyo SEGAWA** (NIMS-LINK)	HYDROGEN GAS SEPARATION OF ORGANIC–INORGANIC HYBRID Si-C MEMBRANES DERIVED FROM POLYCARBOSILANE
19:00-21:00	**Welcome Dinner at La Taverne (https://www.lataverne-rennes.com/)**	
	50 meters from MERCURE Rennes Centre Gare hotel	

Tuesday, JUNE 4 2024		
Time	Speaker	Title
	Session III: Materials for Energy and Environment	
	Chairs: Marielle THIBAULT and Tohru SUZUKI	
08:30-09:10	**Keynote Talk**	
	Samuel BERNARD (IRCER-CNRS)	PDC CHEMISTRY AS A POWERFUL TOOL FOR THE DESIGN OF FUNCTIONAL INORGANIC MATERIALS
09:10-09:25	**Takao MORI** (NIMS-LINK)	GOING ON STRONG: MORE THAN A DECADE OF THERMOELECTRIC COLLABORATION BETWEEN NIMS AND CNRS/LINK
09:25-09:40	**François CHEVIRE** (ISCR-CNRS)	CARBODIIMIDES: ANOTHER CLASS OF N-CONTAINING INORGANIC MATERIALS
09:40-09:55	**Takashi TAKEDA** (NIMS)	ADVANCED PHOSPHORS FOR LIGHTING AND DISPLAYS
09:55-10:15	**Coffee break and Poster session**	
	Chairs: Corinne LAGROST and Takao MORI	
10:15-10:30	**Thierry GACOIN** (Polytechnic-CNRS)	MICROSTRUCTURE AND ANISOTROPY ISSUES IN THE DEVELOPMENT OF NANOCRYSTALS WITH ORIGINAL OR OPTIMIZED OPTICAL PROPERTIES
10:30-10:45	**Soshi IIMURA** (NIMS-LINK)	IONIC AND ELECTRONIC CONDUCTION IN RARE-EARTH METAL OXYHYDRIDES
10:45-11:00	**Tohru SUZUKI** (NIMS-LINK)	MICROSTRUCTURE CONTROL IN BULK CERAMICS BY EXTERNAL FIELDS
11:00-11:15	**Cyril CONDOLF** (SGRP)	DESIGN OF NEW REFRACTORY ALLOYS FOR MOLTEN GLASS PROCESSING
11:15-11:30	**Virginie NAZABAL** (ISCR-CNRS)	CHALCOGENIDE-BASED-MATERIALS FOR OPTICAL SENSOR APPLICATIONS
11:30-11:45	**Barbara BOUTEILLE** (SGRP)	PHASE SEPARATION IN GLASS THIN FILMS FOR SURFACE NANOSTRUCTURATION
11:45-11:50	**Closing remarks by F. TESSIER and J.-F. HALET**	
11:50-13:15	**Lunch buffet**	
13:15	**Move to 10th years anniversary of LINK**	

List of Poster

P.1 PEROVSKITE SOLAR CELLS WITH ADDITIVES AND INTERFACIAL ENGINEERING, Doyeon HEO, NIMS, Tsukuba.

P.2 POLYMER-DERIVED CERAMICS (PDC) ROUTE TOWARDS ENCAPSULATED NON-NOBLE METAL NANOCATALYSTS FOR ALKALINE WATER ELECTROLYSIS, Marwan BEN MILED, IRCER, Limoges.

P.3 INORGANIC ALL-SOLID SOLAR CELLS BASED ON OCTAHEDRAL MOLYBDENUM CLUSTERS, Antoine LEGENDRE, ISCR, Rennes.

P.4 PREDICTION AND DESCRIPTION OF MULTI-COMPONENT CENTERED CUBIC ALLOYS FOR HYDROGEN STORAGE, Zeineb NEFZI, ICMPE, Thiais.

P.5 TRANSITION METAL NITRIDES SYNTHESES FROM METALLIC CLUSTERS: APPLICATIONS TO THE WATER-GAS SHIFT (WGS) REACTION, Sébastien MATHIVET, ISCR, Rennes.

P.6 SOFT PATHWAY FOR MOLYBDENUM CARBIDE AND NITRIDE SYNTHESES: APPLICATION TO THE HYDROGEN EVOLUTION REACTION (HER), Guillaume DUBOIS, ISCR, Rennes.

P.7 IMPROVING VERY HIGH TEMPERATURE THERMOELECTRIC PERFORMANCE OF Yb_4Sb_3 THROUGH DUAL SUBSTITUTIONS: A THEORETICAL STUDY, Vincent PELLETIER, ISCR, Rennes.

P.8 OPTIMIZATION OF THERMOELECTRIC PROPERTIES OF MISFIT LAYERED SULFIDE BY COMPOSITIONAL TUNING, Divyesh PARMAR, IMN, Nantes.

P.9 NOVEL INSIGHTS INTO COMPLEX HYDRIDES FROM GUIDED EVOLUTIONARY STRUCTURE PREDICTION, Vladimir BATURIN, ICMPE, Thiais.