

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)

Ass. Prof. Y. BREARD (Caen Univ.)

Dr. F. GRASSET (LINK, CNRS)

Dr. M. KONO (LINK, SGKK)

Dr. N. OHASHI (NIMS)

Dr. N. SAITO (NIMS)

M. S. PAOFAI (ISCR, UR)

Ms. A. QUEANT-HEMONIN (ISCR, CNRS)

Financial support



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

June 2nd - 4th, 2024

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
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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) (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_xSi₃

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 ELECTROPHORETIC 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: Barbara BOUTEILLE 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 CHARACTERIZATION 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	Virginie NAZABAL (ISCR-CNRS)	CHALCOGENIDE-BASED-MATERIALS FOR OPTICAL SENSOR APPLICATIONS
17:15-17:30	Noriko SAITO (NIMS-LINK)	GAS SENSOR APPLICATIONS OF SEMICONDUCTIVE NANOPARTICLES
17:30-17:45	Marielle THIBAUT (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 THIBAUT 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: Virginie NAZABAL 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	Thierry GLORiant (ISCR-INSA)	OUTSTANDING STRAIN-HARDENING OF A NEW METASTABLE BETA-TITANIUM ALLOY ELABORATED BY IN SITU ADDITIVE MANUFACTURING L-PBF PROCESS
11:30-11:45	Barbara BOUTEILLE (SGRP)	TDB
11:45-11:50	Closing remarks by XXXXX	
11:50-13:15	Lunch buffet	
13:15	Move to 10th years anniversary of LINK	

List of Posters

- 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 SYNTHESSES FROM METALLIC CLUSTERS: APPLICATIONS TO THE WATER-GAS SHIFT (WGS) REACTION, Sébastien MATHIVET, ISCR, Rennes
- P.6 SOFT PATHWAY FOR MOLYBDENUM CARBIDE AND NITRIDE SYNTHESSES: 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