N° 10

News
International Newsletter

December 2018

Editorial

Our citizens are waiting for progress in science and ICMPE is participating in this expansion of knowledge. This year, we achieved new results in the fields of energy storage, advanced or predicted compounds, electro-organic synthesis or sustainable materials. An overview of this cutting-edge research is given in the current newsletter through a selection of recently published articles.

Looking ahead, beside two new ANR projects (Locotherm and Gauguin), we are proud to announce the selection of two young-scientist ANR projects (Camel and Scrin). The recent recruitment of these young scientists give rise to a promising science that we are eager to support.

At the international level, we are participating in a new Franco-Ukrainian LIA on thermostable polymers and in a EU project HyCARE on storage of renewable energies by hydrogen carriers.

Finally, we are involved in science dissemination by organizing the 1st workshop on "Artificial intelligence for materials chemistry", a promising research field.

No doubt that all these actions will be helpful in preparing our institute for our next HCERES peer-review scheduled for early next year.

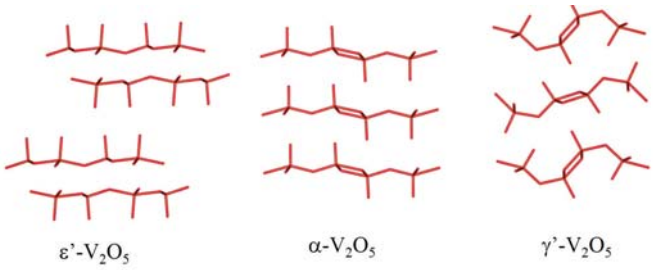
Michel Latroche, director of ICMPE.

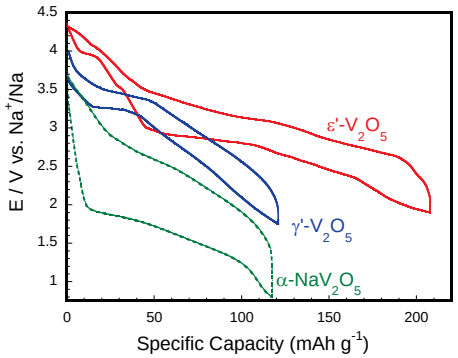
Energy Storage

The richness of V_2O_5 polymorphs as superior cathode materials for sodium insertion

Layered α- ε′- and γ′-V_2O_5 vanadium oxides are evaluated as cathode materials for sodium ion batteries. A full electrochemical and structural reversibility is demonstrated for ε′- and γ′-V_2O_5 compounds at high voltage of 2.8 V. This noticeable voltage enhancement of +1 V compared to Na insertion in α-V_2O_5 is ascribed to the specific structural organization consisting of bilayered and puckered sheets in ε'-V_2O_5 and γ'-V_2O_5, respectively.

These materials constitute new competitive cathode for sodium-ion batteries, able to deliver large capacities (from 120 to 200 mAh g^{-1}) with an outstanding cycling stability over at least 50 cycles.





Layer organization and electrochemical properties of α-, ε′- and γ′-V_2O_5 phases

R. Baddour-Hadjean, M. Safrany Renard, N. Emery, L. T. N. Huynh, M. L. P. Le, J. P. Pereira-Ramos, Electrochim. Acta, 2018, 270, 129-137.

Contact : baddour@icmpe.cnrs.fr

INSTITUT DE CHIMIE ET DES MATERIAUX PARIS-EST

Predicted Materials

Systematic First-Principles Study of Binary Metal Hydrides

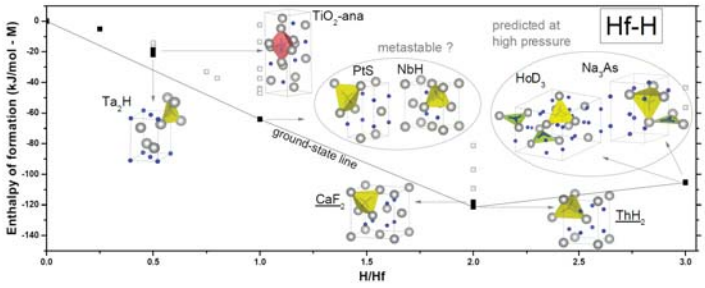
Predicting the formation of reversible metal hydrides is essential in a wide range of environmental issues, such as hydrogen storage for energetic use. In this frame, the enthalpy of formation, ΔH_{for}, is the physical key quantity because it explains the stability of a given hydride relatively to the pure elements.

In this work, first-principles calculations were systematically performed for 31 binary metal−hydrogen (*M*−H) systems (*M* = Hf, Mg…) on a set of 30 potential crystal structures selected on the basis of experimental data and possible interstitial sites (NaCl, CaF_2, ….).

For each *M*−H system, the calculated enthalpies of formation were represented as functions of H composition. The sequence of stable hydrides (ground-state) given by the convex hull was found in satisfactory agreement with the experimental data.

In addition, new high pressure dihydrides and trihydrides were predicted, providing orientations for new materials synthesis.

The overall results provide a global overview of hydride relative stabilities and relevant input data for thermodynamic modeling methods and machine learning algorithms.



N. Bourgeois, J.-C. Crivello, P. Cenedese, and J.-M. Joubert, ACS Comb. Sci., 2017, 19, 513-523.

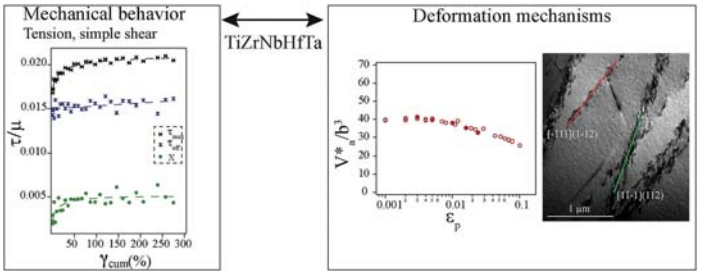
Contact : crivello@icmpe.cnrs.fr

Advanced Materials

Study of a bcc multi-principal element alloy: Tensile and simple shear properties and underlying deformation mechanisms

The impact of a concentrated solid solution on the deformation mechanisms of a bcc multi-principal elements alloy is investigated. The room temperature mechanical properties in tension and simple shear are studied on samples with controlled microstructure. The partition of the various stress components is performed, as well as the determination of the activation volumes and the analysis of the dislocation density and velocity. The study of the mechanical behavior is coupled to a complete TEM investigation.

The alloy displays a high yield strength that is explained by a strong impact of the shortrange obstacles to the dislocation glide, with an enhancement of the effective stress due to the concentrated solid solution. The increase of the backstress is related to the formation of a heterogeneous dislocation structure, with dense dislocation bands acting as long-range obstacles. Deformation is controlled by screw dislocation glide. The a/2<111> screw dislocations are rectilinear, indicating a high lattice friction effect. Evolution of both dislocation velocity and density during multi-relaxation transients suggests a low mobility. If activation volumes are consistent with a Peierls mechanism, other considerations rather head towards the hypothesis of a transitory regime where the solid solution could impact further the dislocation glide.



*L. Lilensten, J.-P. Couzinié, L. Perrière, A. Hocini, C. Keller, G. Dirras, I. Guillot, Acta Mater., 2018, **142**, 131.*

Contact : couzinie@icmpe.cnrs.fr, guillot@icmpe.cnrs.fr

Past events

● On October 5-6 2017, LSPM, ICMPE and the High Pressure Technology Network, organized the "SPS 2017-National Pulse Current Sintering Days" workshop, whose topics focused on material shaping processes through unconventional synthetic routes combining pressure and temperature (112 participants, from France and also Belgium, Germany, Japan and Israel). It was the occasion to celebrate the 10th anniversary of the acquisition of the Spark Plasma Sintering regional apparatus, financed by 10 Ile-de-France laboratories with CNRS support, and to present the future regional platform and the recent acquisition of a high temperature isostatic compaction furnace.

● A workshop on "Artificial Intelligence for materials chemistry" organized by J.-C. Crivello (ICMPE) and N. Sokolovska (UPMC) has taken place on 25 September 2018 at ICMPE with the support of the “CNRS Cellule Énergie”, the PEPS "MaLeFHYCe18" program and the “Fédération pour l'Enseignement et la Recherche en Métallurgie en Ile-de-France, FERMI". Its objective was to bring together French and European actors involved in artificial intelligence (AI) applied to chemistry and materials sciences. With both general and specific presentations, this meeting has gathered 70 participants and has been an opportunity to review the state of the art in this field. Info on https://ai4mater-sci.sciencesconf.org/

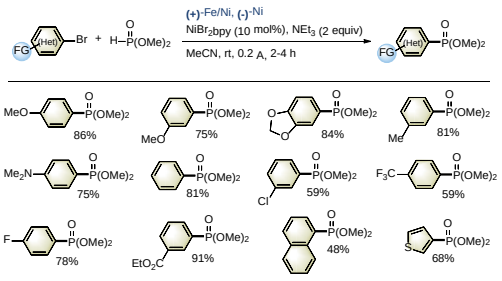
● A workshop dedicated to the chemistry of Cobalt was held at ICMPE on October 12, 2018. Presentations have addressed the role of Co in organic synthesis, batteries, high entropy alloys, Co-based polymers and intermetallic compounds.

Electro-organic synthesis

A mild electroassisted synthesis of (hetero)-arylphosphonates

Electro-organic synthesis has benefited of constant interest in the last decades, since it constitutes a possible alternative to classic organic synthesis, leading to innovative works. The use of reductive electrochemical process in Csp^2-P bonds formation was investigated for the synthesis of (hetero)aromatic phosphorus-containing compounds, which are widespread in materials science or can exhibit many interesting applications in biology and catalysis.

Thus, using the nickel-catalyzed soluble anode process in an undivided cell, various functionalized (hetero)arylphosphonates have been prepared in generally good yields, under mild and simple galvanostatic conditions.



Selected examples of (hetero)arylphosphonates prepared by Csp^2-P electroreductive couplings.

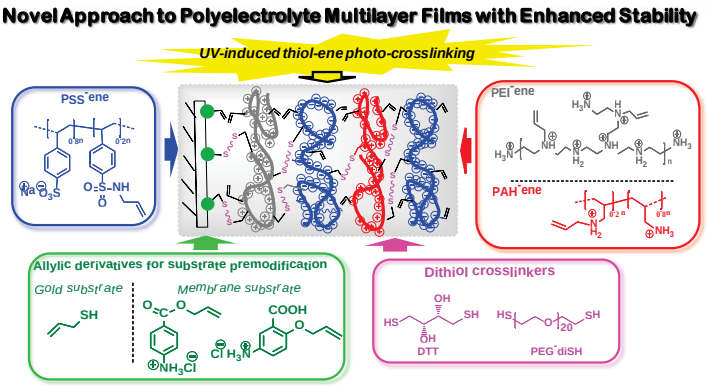
Stéphane Sengmany, Anthony Ollivier, Erwan Le Gall and Eric Léonel, Org. Biomol. Chem., 2018, 16, 4495–4500.

Contact : leonel@icmpe.cnrs.fr

Sustainable Materials

From the functionalization of polyelectrolytes to the development of a versatile approach to the synthesis of polyelectrolyte multilayer films with enhanced stability

A general approach to side-chain allyl-functionalization of three different polyelectrolytes (PEs), namely poly(allylamine) hydrochloride, branched polyethyleneimine, and poly(sodium 4-styrenesulfonate), was reported for the first time. We also demonstrated the application of the resulting allyl-functionalized PEs-ene in the construction of polyelectrolyte multilayer (PEM) films with enhanced stability under harsh conditions, *i.e.* strongly alkaline or acidic solutions or in high ionic strength solutions. One such stability was achieved *via* thiol-ene UV photo-crosslinking between different PE-ene layers and the substrates preliminarily functionalized with allyl functional groups either *via* sulfur–gold chemistry (gold flat substrate) or *via* chemical reduction of aryldiazonium salts using two newly synthesized anilinium derivatives (rough anion-exchage membrane), in the presence of a water-soluble dithiol crosslinker. The versatility and effectiveness of the novel approach presented here is expected to find widespread interest in different fields of emerging applications involving functional organic materials, including advanced membrane separation and purification, antifouling surface engineering, and soft nanotechnology.



T.-T.-T. Nguyen, S. Belbekhouche, P. Dubot, B. Carbonnier D. Grande, J. Mater. Chem., A, 2017, 5, 24472-24483.

Contacts : tnguyen@icmpe.cnrs.fr, grande@icmpe.cnrs.fr

Up-coming workshops and conferences

● ICMPE will host the 9th Workshop "Batteries Lithium en Île-de-France" organized by R. Baddour-Hadjean, J.-P. Pereira-Ramos and G. Bernari (ICMPE GESMAT,) and H. Groult (Sorbonne Université), the 13th of December 2018. Free inscription. *Contact: bernari@icmpe.cnrs.fr*

● The 2018-19 school year has been designated by the Ministries of National Education and of Higher Education, Research and Innovation, Year of Chemistry from School to University, with the support of "Union des Industries Chimiques", CNRS, CEA, SFC, "Fondation de la Maison de la Chimie" and "Comité National de la Chimie". On this occasion, the National Institute of Chemistry (CNRS) will organize on April 3, 2019 a meeting between ICMPE researchers and professors of college and high school through a series of conferences and experimental demonstrations by ICMPE teams.

● ICMPE (D. Grande) along with ICTP (CSIC, Spain) will organize the next Europolymer Conference (EUPOC 2019) on Electrospining and Related Techniques: From Design to Production of Advanced Polymer Materials and Devices (https://www.aim.it/eupoc2019). It will be held in Como (Italy) from May 12 to 16, 2019. The conference will cover the design, characterization and properties of novel electrospun (nano)fibrous polymer and composite materials, as well as their application in various areas (tissue engineering, drug delivery, energy storage, nanotechnology).

Distinctions

Ghada Asskar, a 1st-year PhD student under the supervision of T. Martens (ESO), was awarded for her poster "Zincke salt or Aminopentadienal: which reagent to transform primary amines into pyridinium salts?", presented thanks to the support of her doctoral school at the 17th symposium of the French-American Chemical Society (Orléans, 3-7 June 2018).

Welcoming our new staff members

ICMPE is delighted to welcome Philippe Chevallier as a new permanent CNRS assistant engineer in the team “Métaux et Céramiques à Microstructures Contrôlées” (MCMC). He graduated in Materials Science from Évry University (IUP). He is in charge of mechanical and nano-indentation testing within the ICMPE characterization platform.

We also warmly welcome Dr. Benoît Couturaud, new associate professor of the “Systèmes Polymères Complexes” team and the Chemistry Department (UPEC Technology Institute (IUT) of Chemistry). After his PhD in Materials Chemistry from Montpellier University devoted to polylysine-grafted dendrimers, he has partici-pated as a postdoctoral associate to three separate academic projects dealing with polymer synthesis, in France and abroad (UK and Australia). He was the recipient of an Individual Fellowship from the Marie Curie program. He is currently working in our Institute within the polymer research group, targeting oligomers and polymers displaying bioactive moieties (e.g. oligopeptides) as side substituents, for biomedical applications.

ICMPE acknowledges contributions of its members in writing books, chapters and review articles

M. Laurent-Brocq and J.-P. Couzinié. Issue of *Techniques de l’Ingénieur* (RE269 V1) on « Alliages multi-composants à haute entropie - Concepts, microstructures et propriétés mécaniques. »
https://www.techniques-ingenieur.fr/

R. B. Amar, S. Mahouche-Chergui, A. Oun, M. Khemakhem and B. Carbonnier. “Preparation and surface modification of porous ceramic membranes for water treatment”, Chapter 4, p.101-126, in Advanced Materials for Membrane Fabrication and Modification, CRC Press Taylor & Francis Group, Editors S. Gray, T. Tsuru, Y. Cohen, W.-J. Lau, 2018.
https://www.crcpress.com/

V. Paul-Boncour, A. Percheron-Guégan, M. Latroche, J.-M. Joubert, F. Cuevas *et al.* "Hydrogen Storage Materials". Book in the Landolt-Börnstein collection, E. Burzo, ed., Springer-Verlag, Berlin Heidelberg, 2018.
https://www.springer.com/gb/book/9783662542590

Scientific communication

« Le Journal du CNRS Chine » devotes an article to a Franco-Chinese collaboration between ICMPE (Pr. Valérie Langlois, SPC) and the Center of Synthetic and Systems Biology of Tsinghua University (Pr. George Guo-Qiang CHEN), in the frame of the 2018 ANR SeaBioP project. The common objective is the synthesis of renewable and functional biopolyesters based on new technologies to overcome current challenges, i.e. the reduction of energy and freshwater consumption and the complexity of the fermentation process.

Le CNRS en Chine, N°27/Printemps-été 2018

Nicolas Martin's radio magazine "La Méthode scientifique" from France Culture welcomed Michel Latroche and Bruno Goffé, directors of research at CNRS, as part of its program "Terres rares, le nouvel or noir" broadcast on 24 April 2018. Its purpose was to understand how this extraction industry is organized, how it has been structured in recent years, and how it is beginning to change.

Rare Earths were also the subject of the TV news "20 Heures" broadcast on France 2 with a shooting made within the CMTR team of ICMPE and an interview with Michel Latroche.

New Projects

POLYNANOPOR, a new French-Ukrainian **LIA** on nanoporous thermostable polymers was created on January 2018 (4 years) with CNRS and NASU (Ukraine) financial supports. It involves ICMPE, "Ingénierie des Matériaux Polymères" (Lyon), the Institute of Macromolecular Chemistry (Kiev) and the Institute of Nuclear Research (Kiev). It is coordinated by Dr. D. Grande (ICMPE) and Prof. A. Fainleib (IMC, Ukraine). The aim is to develop thermostable nanoporous hybrid polymer-based films and nanofibers based on high-performance Cyanate Ester Resins, Benzoxazines and Bismaleimides with engineering thermoplastics meant for membrane materials chemically and thermally resistant under severe conditions.

The CMTR team is involved in a new **European project called HyCARE** which focuses on innovative approaches for the storage of renewable energies by hydrogen carriers. It gathers 1 University (UNITO), 4 Research Centres (FBK, HZG, CNRS, IFE) and 4 Industries (ENGIE, GKN, TD, STH). An innovation accelerator for businesses (ENVI) will join UNITO as well as the Korean Lab KIST. The project aims also to engage local authorities, citizens and stakeholders to promote the use of hydrogen as an energy carrier and mutual learning.

Two *Jeunes Chercheuses* ANR projects, **ScrIn**, Screening of ternary intermetallic compounds for themoelectric applications, and **CAMEL**, Chemically architectured metallic alloys, have been respectively awarded to Céline Barreteau (CMTR) and Mathilde Laurent-Brocq (MCMC, with CM Evry as partner).

Other ANR projects for 2018 have also been selected:

"Low Cost Thermoelectric Heuslers Alloys (LoCoThermH)" involving E. Alleno (ICMPE, coordinator) and P. Jund (Institut Charles Gerhardt Montpellier) as principal investigators.

Liquid metal embrittlement occurrence: phenomena and prediction - applied to the Cu-alloys/Ga-In system (Gauguin). ICMPE: E. Leroy, J. Bourgon, L. Perrière. Partners: UMET (coordinator), PIMM, MSSMAT.

ICMPE News

Publisher : **Michel Latroche**
Coordination : **Stéphane Bastide**
Mise en page et Impression : **Nicolas Boisseau**
→ To subscribe, contact: newsletter@icmpe.cnrs.fr

ICMPE
2-8, rue Henri Dunant
94320 Thiais - FRANCE
Tel: +33 (0)1 49 78 11 81
Fax: +33 (0)1 49 78 11 66
http://www.icmpe.cnrs.fr