

PROGRAM

Tuesday 27 March

8:00 *Registration and welcome coffee*

8:45 **Welcome address**

X. Longaygue (Scientific Division, IFPEN) and M. Coral Valero (Catalysis and Separation Division of IFPEN, SLIMAIA scientific correspondent)

SESSION 1: CHARACTERIZATION

Chaired by Marie-Pierre Gaigeot (University of Evry-LAMBE) and Loïc Barré (IFPEN)

9:00 **Keynote: Towards understanding the mechanism of water splitting on TiO₂**
E. H. G. Backus (Max Planck Institute for Polymer Research, Germany)

9:40 **Control of the particle surface charge and the size by polyelectrolyte adsorption at solid-liquid interface**
A. Jada (IS2M, CNRS, UHA, France)

10:00 **Characterization of the non-uniform concentration profile of binary fluids confined in mesopores by neutron scattering methods**
R. Mhana^{1,2}, A. R. Abdel Hamid¹, S. Dutta¹, R. Lefort¹, L. Noirez³, F. Porcher³, C. Alba-Simionesco³, B. Frick², D. Morineau¹ (1 Institute of Physics of Rennes, CNRS, Univ. of Rennes 1 ; 2 Institute Laue-Langevin ; 3 Lab. Léon Brillouin, CEA-CNRS, France)

10:20 *POSTER SESSION / break*

10:50 **Second harmonic scattering: a tool to study at the nanometer-scale the molecular adsorption at materials interfaces**
G. Martin-Gassin, P. M. Gassin, S. Bellini, B. Prelot, J. Zajac (ICGM, CNRS, Montpellier Univ., France)

11:10 **Second harmonic generation at liquid interfaces to probe molecular organization, chirality and complexation**
E. Benichou, O. Bonhomme, P.F. Brevet (Institut Lumière Matière, UMR CNRS 5579, Univ. Lyon 1, France)

11:30 **Molecular investigation of the preparation of alumina-supported co catalysts through an aqueous-phase surface science approach**
C. Schlaup¹, A. Davantès¹, G. Lefevre¹, X. Carrier¹ (1 Sorbonne Univ., UPMC, Réactivité de Surface Lab. ; 2 PSL Research Univ., Chimie ParisTech, CNRS, Institut de Recherche de Chimie Paris, France)

11:50 **Real-time measurement of silica dissolution at the interface with water**
J. Schaefer, E. H. G. Backus, M. Bonn (Max Planck Institute for Polymer Research, Germany)

12:10 **Adsorption of anionic surfactants on silica studied by the quartz-crystal microbalance with dissipation monitoring (QCM-D)**
J. Wolanin, D. Bauer, D. Frot, C. Dalmazzone (IFPEN, France)

12:30 *Lunch*

SESSION 2 : THEORY

Chaired by James Kubicki (University of Texas El Paso) and Pascal Raybaud (IFPEN)

14:00 **Keynote : Water at surfaces**
A. Michaelides (Thomas Young Centre, Univ. College of London, UK)

14:40 **Mineral/water interfaces characterized by ab initio molecular dynamics: making the link between structure and SFG vibrational spectroscopy**
S. Pezzotti, L. Potier, F. Siro Brigiano, D.R. Galimberti, A. Cimas, M-P. Gaigeot (Lab. Analyse et Modélisation pour la Biologie et l'Environnement, Évry Val d'Essonne Univ., Paris Saclay Univ., France)

15:00 **A reaxFF molecular dynamics study of the reactivity between a biodiesel surrogate and the γ -alumina surface**
B. Darenne¹, M. Alves Fortunato¹, D. Costa², T. De Bruin³ (1 IFPEN, Institut Carnot IFPEN Transports Energies ; 2 Lab. de Physico-Chimie des Surfaces, UMR CNRS-ENSCP 7045, ENSCP, Chimie-ParisTech ; 3 IFPEN, France)

15:20 **A force field for water over Pt(111): development, assessment and comparison**
S. N. Steinmann¹, R. Ferreira De Moraes¹, A. W. Götz², P. Fleurat-Lessard³, P. Sautet⁴, C. Michel¹ (1 Univ. of Lyon, ENSL, CNRS, Univ. of Lyon 1, Lab. de Chimie, France ; 2 San Diego Supercomputer Center, Univ. of California, USA ; 3 ICMUB, France ; 4 Dept. of Chemical and Biomolecular Engineering, Univ. of California, USA)

15:40 *POSTER SESSION / break*

16:20 **Blue energy and desalination with nanoporous carbon electrodes: from molecular simulations to continuous models**
N. Ganfoud¹, M. Simoncelli², M. Salanne^{1,2,3}, B. Rotenberg^{1,3} (1 Sorbonne Univ., UPMC, Lab. PHENIX ; 2 Maison de la Simulation, CEA, CNRS, Univ. Paris Sud, UVSQ Univ. Paris Saclay ; 3 RS2E, CNRS, France)

- 16:40 **Adsorption of the complex on the TiO₂(110) surface in presence of water: ab initio molecular dynamics studies**
F. Chiter, A. Tougeri, S. Cristol, J-F. Paul (Lille Sciences et Technologies Univ., CNRS, Unité de Catalyse et Chimie du Solide, France)
- 17:00 **Molecular views on surface-driven flows: the case of thermo-osmosis**
L. Fu, S. Merabia, L. Joly (Claude Bernard Lyon 1 Univ., CNRS, Institut Lumière Matière)
- 17:20 **Computational study on membrane-solute interactions in desalination systems using ion exchange membranes**
A. Fuoco², H. Roux De Balmann¹, S. Galier¹, G. De Luca² (Lab. de Génie Chimique, Univ. of Toulouse, CNRS, INPT, UPS, France ; 2 Istituto per la Tecnologia delle Membrane, C/O Univ. della Calabria)
- 17:40 *End of the presentations*

Wednesday 28 March

- 8:30 *Registration and welcome coffee*

SESSION 3: HETEROGENEOUS CATALYSIS AND SEPARATION

Chaired by Angelos Michaelides (University College of London) and Mickaël Rivallan (IFPEN)

- 9:00 **Keynote: Solid-liquid interfaces in catalysis**
K. P. de Jong (Debye Institute of Nanomaterials Science, Utrecht Univ., The Netherlands)
- 9:40 **From the gas phase to liquid phase: key parameters in transesterification reaction**
D. Cornu, L. Lin, M. Mounir Daou, M. Jaber, J-M. Krafft, V. Herledan, G. Laugel, Y. Millot, H. Lauron-Pernot (Lab. de Réactivité de Surface, CNRS, UPMC, Sorbonne Univ.)
- 10:00 **Aqueous-phase preparation of model HDS catalysts on alumina wafers: surface-dependent speciation of the active phase**
C. Bara^{1,2}, A-F. Lamic-Humblot¹, E. Devers², M. Digne², G. D. Pirngruber², X. Carrier¹ (1 Sorbonne Univ., UPMC, CNRS, Lab. de Réactivité de surface ; 2 IFPEN, France)
- 10:20 *POSTER SESSION / break*
- 10:50 **A study of the organic extraction layer in hybrid mesoporous silica designed for uranium extraction from sulfuric acid medium**
T. Le Nedelec^{1,2}, F. Calard¹, F. Cuer², A. Leydier¹, A. Grandjean¹ (1 CEA, DEN, MAR, DE2D, SEAD, LPSD ; 2 CEA, DEN, MAR, DRCP, SMCS, LDPS, France)

- 11:10 **Ab initio molecular dynamics of acetic acid and ethylene glycol at the water/ γ -alumina interface**
B. F. Ngouana Wakou, M. Corral Valero, P. Raybaud (IFPEN, France)
- 11:30 **An in-situ spectroscopic study at the solid-liquid interface of co-adsorption of co-carboxylate complexes on gamma alumina**
G. Lefèvre¹, A. Davantès¹, C. Schlaup², X. Carrier², M. Rivallan³ (1 PSL Research Univ., Chimie ParisTech, CNRS, Institut de Recherche de Chimie Paris ; 2 Sorbonne Univ., UPMC, UMR CNRS 7197, Lab. de Réactivité de Surface ; 3 IFPEN)
- 11:50 **In situ and operando IR spectroscopy for investigation of solid-liquid Interfaces during fuel purification by adsorption or catalytic processes**
I. Khalil¹, C. Celis-Cornejo², V. G. Baldovino-Medrano², J-F. Paul³, K. Thomas¹, A. Travert¹, F. Maugé¹ (1 Normandie Univ., Unicaen, CNRS, Lab. Catalyse et Spectrochimie ; 2 UIS, Centro de Investigaciones en Catálisis, Colombia ; 3 Lille Univ., CNRS, ENSCL, Unité de Catalyse et de Chimie du Solide)
- 12:10 **A first-principles investigation of fluorination at the TiO₂(001)/H₂O solid-liquid interface**
K. G. Reeves¹, D. Dambournet¹, C. Laberty-Robert², R. Vuilleumier³, M. Salanne¹ (1 Sorbonne Univ., UPMC, CNRS, PHENIX ; 2 Sorbonne Univ., UPMC, CNRS, Collège de France, Lab. de Chimie de la Matière Condensée de Paris ; 3 Sorbonne Univ., UPMC, ENS, CNRS, Pasteur)

12:30 *Lunch*

SESSION 4 : GEOCHEMICAL AND ENVIRONMENTAL ISSUES

Chaired by Gregory Lefevre (CNRS-PSL) and Xavier Carrier (LRS-PSL)

- 14:00 **Keynote: Quantum mechanical modeling of mineral-water interfaces with surface defects**
J. D. Kubicki (Dept. of Geological Sciences, Univ. of Texas, USA)
- 14:40 **Adsorption and retardation of organic molecules: past and new insights on hydrophilicity**
R.V.H. Dagnelie (SECR, CEA, Univ. of Paris-Saclay, France)
- 15:00 **Adsorption of anionic surfactant on non-swelling clays**
A. Suzzoni^{1,2}, L. Barré¹, É. Kohler¹, P. Levitz², L. Michot² (1 IFPEN ; 2 PHENIX, UPMC, France)
- 15:20 *POSTER SESSION / break*
- 16:20 **Innovation in sorption processes: from the understanding of interaction mechanisms to the design of original sorbents**
U. Dong Thach, G. Darmograi, A. Geneste, P. Hesemann, G. Gassin, J. Zajac, B. Prelot (ICGM, CNRS, Univ. of Montpellier, France)

- 16:40 **Furthering our understanding of solvated interfaces by integrating calorimetry-based experimental thermodynamics and computational approaches**
A. Namayandeh¹, N. Allen¹, P. Ilani Kashkoul¹, H. Watts², J. Kubicki², N. Kabengi^{1,3}
(1 Dept. of Geosciences, Georgia State Univ. ; 2 Dept. of Geological Sciences, Univ. of Texas ; 3 Dept. of Chemistry, Georgia State Univ., USA)
- 17:00 **Development of selective materials for removing cesium and strontium from contaminated liquid**
Y. Barre , A. Hertz, C. Guevar, A. Grandjean (CEA, DEN, DE2D, SEAD, LPSD, France)
- 17:20 **Keynote: Reflections on the solid/liquid interface**
S. Clarke (BP Institute and Department of Chemistry, Univ. of Cambridge, UK)
- 18 :00 *End of the presentations*
Departure to the Château de La Malmaison for the guided visit and the dinner

Thursday 29 March

8:30 *Registration and welcome coffee*

SESSION 5 : ELECTROCHEMISTRY AND CORROSION

Chaired by Bénédicte Prélot (CNRS-ICG) and Theodorus de Bruin (IFPEN)

- 9:00 **Keynote: Electrode/electrolyte interface in porous electrode materials for electrochemical capacitor applications**
P. Simon (Paul Sabatier Univ., Cirimat, CNRS, RS2E, Institut universitaire de France, France)
- 9:40 **Energy storage upon forced intrusion of a nonwetting fluid in a (meso, nano) porous material. A high T & P scanning transitiometric investigation**
J-P. E. Grolier¹, Y. Grosu² (1 ICCF Univ. of Auvergne, CNRS, SIGMA, France ; 2 CIC Energigune Albert Einstein, Spain)
- 10:00 **Methodology to measure the local pH in aqueous CO₂ corrosion**
R. de Motte¹, R. Mingant¹, J. Kittel¹, F. Ropital¹, P. Combrade², S. Necib³, V. Deydier³, D. Crusset³ (1 IFPEN ; 2 Acxcor ; 3 Andra, France)
- 10:20 *Break*
- 10:40 **Electrochemical property of microporous supercapacitor by classical density functional theory**
L. Qing¹, S. Zhao¹, H. Liu², Y. Hu² (1 School of Chemical Engineering, East China Univ. of Science and Technology ; 2 School of Chemistry and Molecular Engineering, East China Univ. of Science and Technology, China)

- 11:00 **In-situ study of interfacial bonding degradation of polyester coating on multi-metal oxides**
L. I. Fockaert^{1,2,3}, S. Pletincx⁴, H. Terryn^{3,4}, J. M. C. Mol³ (1 Netherlands Organisation for Scientific Research ; 2 M2i ; 3 Delft Univ. of Technology, Dept. of Materials Science and Engineering, The Netherlands ; 4 Vrije Univ. of Brussel, Research Group Electrochemical Surface Engineering, Belgium)
- 11:20 **Demistifying corrosion inhibition and lubrication: application of atomistic computational methods to benzotriazole and friction modifiers**
C. Gattinoni, J. Ewen, A. Michaelides, D. Dini (Materials Theory, Dept. of Materials, ETH Zürich, Switzerland)
- 11:40 **Quartz crystal microbalance with dissipation (QCM-D) as a new wettability characterization tool: its challenges and how they were resolved**
S. Erzuah^{1,2}, I. Fjelde^{1,2,3}, A. Voke Omekeh^{1,3} (1 Univ. of Stavanger – UIS ; 2 National IOR Centre of Norway ; 3 International Research Institute of Stavanger - IRIS, Norway)
- 12:00 **Electro-osmosis: a simple description from an analysis at the molecular level**
B. Siboulet¹, J-F. Dufreche¹, R. Hartkamp² (1 ICSM/LMCT, UMR 5257, CEA, Univ. of Montpellier, ENSCM, CNRS, France ; 2 Process and Energy Dept. Delft Univ. of Technology, The Netherlands)
- 12:20 **Conclusion and highlights of the SLIMAIA conference** by Manuel Corral Valero, scientific correspondent of this *Rencontre scientifique*
- 12:30 *Lunch*



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