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- P73 Kinetic study on iron oxides' redox transformations under secondary conditions of nuclear power pressurized water reactor**
Z. Li^{1,3}, G. Lefevre¹, C. Chaneac², S. Delaunay³, A. Graff³ (1 PSL Research Univ., Chimie ParisTech, CNRS, Institut de Recherche de Chimie ; 2 Sorbonne Univ., UPMC, CNRS, Collège de France, LCMCP ; 3 EDF Research and Development, France)
- P81 Insight by operando tem on the thermal behaviour of cobalt-based fischer-tropsch catalysts**
K. Dembélé^{1,2}, M. Bahri^{1,2}, C. Hirlimann¹, G. Melinte¹, S. Moldovan, A. Berliet², A.-S. Gay², S. Maury², O. Ersen^{1,3,4} (1 IPCMS, Univ. de Strasbourg, CNRS ; 2 IFPEN ; 3 USIAS, 4 IUF, France)
- P85 Determination of the surface charge of the water-solid surface at low and high pH**
S. Sun, M. Bonn, E. H. G. Backus (Max Planck Institute for Polymer Research, Germany)
- P88 Application of inverse liquid chromatography to the surface characteristics of mesoporous aluminosilicates**
K. Adamska, A. Voelkel (Institute of Chemical Technology and Engineering, Poznan Univ. of Technology, Poland)
- P95 Air/water and silica/water interfaces characterized by ab initio molecular dynamics**
S. Pezzotti^{1,2}, D. R. Galimberti^{1,2}, F. S. Brigiano^{1,2}, M-P. Gaijeot^{1,2} (1 LAMBE, Univ. D'Evry Val d'Essonne, 2 Univ. Paris-Saclay, France)
- P96 Aqueous surface science: R-(1102) alpha-alumina in the presence of bulk liquid water**
L. Potier^{1,2}, S. Pezzotti^{1,2}, A. Cimas^{1,2}, M-P. Gaijeot^{1,2} (1 LAMBE, Univ. d'Evry val d'Essonne, 2 Univ. Paris-Saclay, France)
- P97 Amorphous silica/water interfaces from DFT-MD simulations and VSFG spectroscopy**
F. S. Brigiano^{1,2}, S. Pezzotti^{1,2}, M-P. Gaijeot^{1,2} (1 LAMBE, Univ. d'Evry val d'Essonne, 2 Univ. Paris-Saclay, France)

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- P6 Calculation of a solid/liquid surface tension: a methodological study**
T. Dreher^{1,2}, C. Lemarchand¹, L. Soulard¹, E. Bourasseau³, P. Malfreyt², N. Pineau¹ (1 CEA/DAM/DIF, 2 Univ. Clermont Auvergne, CNRS, ICCF, Sigma, 3 CEA/DEN/DEC, France)
- P12 Surface wettability effect on molecular morphology, transport and reaction**
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)
- P15 Classical density functional theory of capacitors for blue energy applications**
S. W. Coles¹, N. Ganfoud¹, M. Salanne^{1,2}, G. Jeanmairet¹, B. Rotenberg^{1,3} (1 Sorbonne Univ., UPMC, CNRS, PHENIX ; 2 Maison de la Simulation, CEA, CNRS, INRIA, Univ. Paris-Sud, Univ. de Versailles ; 3 RS2E, France)
- P51 Computational study of mea adsorption on hydroxylated CR₂O₃ surface**
T. De Bruin¹, A. Gouron^{1,2}, A.C.T. Van Duin³, D. Van Duin³, B. Diawara², F. Ropital⁴ (1 Dept. of Thermodynamics and Molecular Modeling, IFPEN, 2 Institut de Recherche de Chimie Paris, CNRS, Chimie ParisTech, France ; 3 RxFF Consulting, LLC, State College, USA ; 4 Dept. of Electrochemistry and Materials, IFPEN, France)
- P74 Developing an efficient approach for the computation of free solvation energy at the metal / liquid interface**
P. Clabaut, B. Schweitzer, C. Michel, S. Steinmann (Univ. Lyon 1, École Normale Supérieure de Lyon, CNRS, Lab. de Chimie, France)
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- P90 Adsorption of hydroxydes on graphene and H-BN single layers in water**
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- P92 Stabilisation and isomerisation of formic acid at a mineral/water interface**
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- P93 Adsorption of water and glycine on rutile (110) surface, a DFT-D approach including implicit and explicit solvent**
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- P94 First-principles molecular dynamics (FPMD) simulations of CO₃O₄/aqueous solutions interfaces: electrocatalysis & water splitting**
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A. C. Bueno^{1,2}, Y. Schuurman², M. Klotz¹, D. Farrusseng²
(1 Saint-Gobain CREE, Lab. de Synthèse et Fonctionnalisation des Céramiques, CNRS, 2 IRCELYON, Institut de recherches sur la catalyse et l'environnement, CNRS, France)
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- P30 The influence of nature and the content of silica on the synthesis of isostructural silicoaluminophosphate chabasite SAPO-34**
S. Bellatreche^{1,2}, M. A. Hasnaoui², A. Bengeddach² (1 Faculty of Medicine, Univ. d'Oran ; 2 Lab. de chimie des matériaux, Univ. of Oran, Algeria)
- P43 Ab initio molecular dynamics study of the γ -alumina / water interface**
B. F. Ngouana Wakou¹, P. Cornette², M. Corral Valero¹, D. Costa², P. Raybaud¹ (1 IFPEN ; 2 Physico-Chimie des Surfaces, PSL Research Univ., CNRS, Institut de Recherche de Chimie Paris, Chimie ParisTech, France)
- P64 Heterogeneous autocatalytic reactions: towards a macroscopic model of reactors for the dissolution of uranium dioxide**
S. Lalleman¹, F. Charlier¹, A. Magaldo¹, P. Marc¹, G. Borda¹, É. Schær² (1 CEA, Nuclear Energy Division, Research Dept. of Mining and Fuel Recycling Processes ; 2 Lab. of Reaction and Process Engineering, CNRS, Univ. of Lorraine, France)

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- P8 Interactions of divalent cations with hydrated clay particles edges**
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- P18 Adsorption in flow conditions**
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- P58 Comparative study of the retention mechanisms of strontium and cesium on zeolites**
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- P91 The role of activation in the recovery of copper from chalcopyrite ore during the FLSmidth® ROL process**
A. P. Karcz¹, A. Juul Damø¹, K. Dam-Johansen¹, D. Chaiko² (1 The Technical Univ. of Denmark, Denmark, 2 FLSmidth® Minerals, U.S.A)

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I. Benmahammed¹, T. Douadi¹, S. Issaadi² (1 LEMMC, Dept. de Génie des Procédés, Faculté de Technologie, Univ. Ferhat Abbas Sétif-1 ; 3 Faculté des Sciences, dept. de Chimie, Univ. Ferhat Abbas Sétif-1, Algeria)
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- P29 Stabilization of magnetite aqueous dispersion by PS-PEO copolymer and its use as adsorbent for remediation of metal ions in polluted water**
I. Hachilif, A. Jada (IS2M, CNRS UHA, France)
- P31 Mesoscopic lattice-based simulation to account for electrokinetic and adsorption/desorption effects**
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- P47 Electrochemical treatment of wastewater containing cresol**
Z. Taleb¹, E. Morallón², R. Berenguer³, C. Quijada⁴, S. Taleb¹ (1 Lab. of Materials & Catalysis, Faculty of Exact Sciences, Djillali Liabes Univ., Algeria ; 2 Instituto Univ. de Materiales, Dept. de Química Física, Univ. of Alicante, 3 Univ. of Málaga, Dept. de Ingeniería Química, 4 Dept. de Ingeniería Textil y Papelera, Univ. Politècnica de València, Spain)
- P53 The use of doped conducting polymers for supercapacitors**
D. Amoura¹, M. Sanchez-Jiménez², F. Estrany^{2,3}, L. Makhloufi¹, C. Aleman^{3,4} (1 LECVE, Faculté de Technologie, Univ. of Bejaia, Algeria ; 2 Dept. d'Enginyeria Química, Escola Univ. d'Enginyeria Tècnica Industrial de Barcelona, Univ. Politècnica de Catalunya ; 3 Center for Research in Nano-Engineering, Univ. Politècnica de Catalunya, 4 Dept. d'Enginyeria Química, ETS d'Enginyers Industrials, Univ. Politècnica de Catalunya, Spain)
- P79 Electrochemical synthesis of a 1-cyano-tetrahydroisoquinoline**
F. Louafi¹, J-P. Hurvois², L. Benmekhbi¹, A. Chibani¹ (1 Univ. of Constantine1, Dept. de Chimie, Algeria ; 2 Sciences chimiques de Rennes, CNRS, Univ. of Rennes 1, France)

