



Computational chemistry for pollutant mitigation

Rueil-Malmaison (near Paris) France ■ 13-14 March 2017

Monday 13 March

8.15 Registration

9.00 Welcome Address
Xavier Longaygue, Scientific Division (IFPEN, France)

Opening of the conference
Theodorus de Bruin, Scientific correspondent of Computational Chemistry conference (IFPEN, France)

SESSION 1: COMBUSTION AND ATMOSPHERIC CHEMISTRY

9.10 Keynote Lecture by **Laurence Rouil** (Ineris, France)
Challenges in atmospheric chemistry

9.55 Modelling of iodine atmospheric chemistry
A. Villard^{1,4}, S. Khanniche^{1,4}, C. Fortin^{1,4}, D. Khiri^{1,4}, V. Fèvre-Nollet^{1,4}, P. Lebègue^{1,4}, L. Cantrel^{3,4}, F. Cousin^{3,4}, I. Černušák², F. Louis^{1,4} (1 Univ. of Lille 1, CNRS, France; 2 Department of Physical and Theoretical Chemistry, Slovakia; 3 Institut de Radioprotection et de Sûreté Nucléaire, France; 4 Laboratoire de Recherche Commun IRSN-CNRS-Lille 1, France)

10.20 Thermal destruction of chemical warfare agents
J.-C. Lizardo-Huerta¹, B. Sirjean¹, L. Verdier², R. Fournet¹, P.-A. Glaude¹ (1 Laboratoire Réactions et Génie des Procédés, CNRS, Univ. of Lorraine, France; 2 DGA Maîtrise NRBC, France)

10.45 Break and poster session

11.10 Keynote Lecture by **Angela Violi** (University of Michigan, USA)
Topical review : Challenges in soot formation chemistry

11.55 Formation of the first aromatic ring in 1,3 butadiene combustion
C. Huang^{1,2}, B. Yang¹, F. Zhang² (1 Center for Combustion Energy and Key Laboratory for Thermal Science and Power Engineering of MOE, P.R. China; 2 National Synchrotron Radiation Lab., Univ. of Science and Technology of China, P.R. China)

12.20 Computational chemistry in the automatic generation of combustion kinetic models
V. Warth, B. Sirjean, P.A. Glaude, R. Fournet (Lab. Réactions et Génie des Procédés, CNRS, France)

12.45 Lunch

14.15 Flash communications of posters

SESSION 2: INDUSTRIAL SESSION

15.00 Atomistic Modelling: An Industrial Perspective

M. Sarwar, J. Collier, L. Mantarosie, K. Simmance, A. Martinez, S. French, S. Garcia, S. Ball, X.Xia, G.Jones, Dave Thompsett (Johnson Matthey Technology Centre, UK)

A Cleaner World with MedeA

X. Rozanska (Materials Design, SARL, France)

Reaction Chemistry & Material Properties with the ADF Modeling Suite

T. M. Soini (Software for Chemistry & Materials, The Netherlands)

Carbon Dioxide Adsorption in Polymer Membranes and Microporous Amorphous Carbon

R. Chaudret, A. Bick, S. Schweizer, X. Krokidis (Scienomics, France)

15.50 Break and poster session

SESSION 3: HETEROGENEOUS CATALYSIS

16.15 Keynote Lecture by **William Schneider** (Univ. of Notre Dame, USA)

Topical review: Challenges in environmental catalysis

17.00 DFT study of H₂O and NH₃ coordination capacity at copper in Cu-SSZ-13

B. Kerkeni^{1,2}, D. Berthout¹, D. Berthomieu³, C. Chizallet¹ (1 IFPEN, France; 2 Faculté des Sciences de Tunis, Tunisia; 3 Institut Charles Gerhardt Montpellier, France)

17.25 A combined molecular dynamics and quasi-elastic neutron scattering (QENS) study of diffusion in zeolites

A.J. O'Malley^{1,2,3}, I. Hitchcock⁴, M. Sarwar⁴, I.P. Silverwood⁴, S. Hindocha⁴, C.R.A. Catlow^{1,2}, A.P.E. York⁴, P. J. Collier^{2,4}

(1 Univ. College London, UK; 2 UK Catalysis Hub, UK; 3 ISIS Facility, UK; 4 Johnson Matthey Technology Centre, UK)

17.50 A multiscale approach applied to oxygen adsorption and oxidation reactions on Pt₁₃/γ-Al₂O₃ clusters

A. Sangnier¹, C. Chizallet¹, A. Nicolle¹, C. Dujardin² (1 IFPEN; 2 Univ. of Lille, France)

18.15 Simulation of perovskite materials in emissions control catalysis

C. S. Cooper^{1,2}, M. Sarwar¹, K. Simmance¹, A.P.E. York¹, C.R.A. Catlow²
(1 Johnson Matthey Technology Centre, UK; 2 Univ. College London, UK)

19.00 Bus transfer to the “*Domaine de Vert-Mont*” in Rueil-Malmaison

19.30 Cocktail reception

22.00 Bus transfer from the “*Domaine de Vert-Mont*” to the hotels in Rueil-Malmaison and to “*Place Charles de Gaulle-Etoile*” in Paris

Tuesday 14 March

8.30 Registration

9.00 Plenary Lecture by **William A. Goddard** (Caltech., USA)

Advances in multiscale methods for environmentally-friendly design

9.45 Round Table “Challenges for pollutant mitigation: under-searched areas, human-machine interactions, first-principle based design”

SESSION 4: PLASMA CHEMISTRY

11.15 Break and poster session

11.35 Keynote by **Annemie Bogaerts** (Univ. of Antwerp, Belgium)
Topical review: Challenges in plasma chemistry

12.20 Classical molecular dynamics simulations of plasma sputtered catalyst growth and plasma-catalysis
P. Brault¹, E. C. Neyts² (1 GREMI, CNRS Univ. of Orléans, France; 2 Department of Chemistry, Univ. of Antwerp, Belgium)

12.45 Non equilibrium vibrational and free electron kinetics in CO₂/CO discharges
L. D. Pietanza, G. Colonna, A. Laricchiuta, G. D’Ammando, M. Capitelli (CNR Nanotec, Plasmi Lab., Italy)

13.10 Closing remarks by André Nicolle, Scientific correspondent of Computational Chemistry conference (ENSTA ParisTech, France)

13.20 End of the conference

Poster session

Simulation of aerosol dispersion in southeast Asia using WRF-chem model

S. Pamungkas¹, N. J. Trilaksono¹ (1 Weather and Climate Prediction Lab., Indonesia)

Interaction of ozone with KI aerosols

F. Allouti^{1,4}, S. Souvi^{2,4}, A. Markovits³, F. Louis^{1,4} (1 Univ. of Lille 1; 2 Institut de Radioprotection et de Sûreté Nucléaire (IRSN); 3 Lab. de Chimie Théorique, UPMC 6; 4 Lab. de recherche commun IRSN-CNRS-Lille 1, France)

Temperature and pressure-dependent rate coefficients for C₆H₅+C₂H₂ reaction network

Z. Wang, F. Zhang (National Synchrotron Radiation Lab., Univ. of Science and Technology of China, P.R. China)

First approach for acetone decomposition kinetics in plasmas of atmospheric gases

N. Blin-Simiand, B. Bournonville, L. Magne, S. Pasquiers (Univ. of Paris-Sud, France)

Plasma catalysis at the nanoscale: Model development for diffusion and chemical reactions in catalyst pores

Y. Engelmann, A. Bogaerts, E. C. Neyts (Research Group Plasmant, Belgium)

Self-organization of filaments in the tube by the gas

M. V. Dementieva¹, E. B. Markova^{1,2} (1 Rudn Univ.; 2 Frumkin Institute of Physical Chemistry and Electrochemistry RAS, Russia)

Ab initio mechanistic and thermochemical study of the adsorption of phenanthrene over a hydrocracking catalyst

C. M. Celis-Cornejo, M. M. Garnica-Mantilla, V. G. Baldovino-Medrano, G. E. Ramírez-Caballero (Universidad Industrial de Santander, Colombia)

Preparation and characterization of Co_x Fe_(3-x) O₄/S (S= SiO₂, Al₂ O₃ and MgO and their catalytic activities in total oxidation of ethanol

Y. Hammiche-Bellal, L. Meddour-Boukhobza (Lab. des Matériaux Catalytiques et Catalyse en Chimie Organique, Algeria)

How oxygen vacancies activate CO₂ dissociation on TiO₂ anatase (001)

S. Huygh, Y. Engelmann, A. Bogaerts, E. C. Neyts (Research Group Plasmant, Belgium)

The surface chemistry of methan derived radicals on anatase (001) and the influence of oxygen vacancies

S. Huygh, A. Jafarzadeh, A. Bogaerts, E. C. Neyts (Research Group Plasmant, Belgium)

Oxidative heterogeneous catalytic disposal of chlorinated hydrocarbons

D. Tagiyev^{1,2}, A. Efendi¹, E. Babayev¹ (1 Institute of Catalysis and Inorganic Chemistry named after M. Nagiyev, National Academy of Sciences of Azerbaijan; 2 Azerbaijan Medical Univ.)

The kinetic study of cyanide removal by oxidation with hydrogen peroxide in presence of activated carbon as catalyst

S. Chergui¹, A. R. Yeddou^{1,2}, F. Halet^{1,2}, A. Chergui^{1,3}, B. Nadjemi¹, A. Oulddris⁴ (1 Ecole Normale Supérieure Kouba; 2 Univ. M'Hamed Bougara; 3 Ecole Nationale polytechnique d'Alger, Algeria; 4 Univ. de Technologie de Compiègne, France)

Catalytic oxidation of n-butanol over platinum supported mesoporous silica CMI-1

S. Sabour¹, C. Especel², C. Fontaine², M. Bidaoui³, L. Benatallah¹, N. Bouchenafa-Saib¹, J. Barbier Jr², O. Mohammedi¹ (1 Chimie-Physique des Interfaces des Matériaux Appliquées à l'Environnement, Algeria; 2 Univ. de Poitiers, Institut de Chimie des Milieux et des Matériaux, France; 3 Centre Univ. de Tissémsilt, Institut des Sciences et Technologies, Algeria)

Numerical study of CO₂ adsorption on the activated carbon: role of disordered network, size effect and temperature

D. Nguemalieu Kouetcha¹, H. Ramézani², N. Cohaut¹ (1 Univ. Orléans, France; 2 Ecole Polytechnique de l'Univ. Orléans, France)

Distinctive kinetics on NiZn bimetallic catalysts for hydrogen evolution via selective dehydrogenation of methylcyclohexane to toluene

A. Jedidi¹, A. H. Al-ShaikhAli², Dalaver H. Anjum², L. Cavallo², K. Takanabe² (1 King Abdulaziz Univ.; 2 King Abdullah Univ. of Science and Technology, Saudi Arabia)

Generation of soot basal structure units with ReaxFF

M. Keller¹, T. de Bruin¹, A. Nicolle² (1 IFPEN; 2 Paris-Saclay Univ. / ENSTA Paris Tech, France)