



# 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

*Chairmen: M. Matrat (IFPEN, France) and A. Nicolle (ENSTA ParisTech, France)*

9.10 Keynote Lecture by **Laurence Rouïl** (INERIS, France)

**Challenges in atmospheric chemistry**

9.55 **Modelling of iodine atmospheric chemistry**

A. Villard<sup>1,4</sup>, S. Khanniche<sup>1,4</sup>, C. Fortin<sup>1,4</sup>, D. Khiri<sup>1,4</sup>, V. Fèvre-Nollet<sup>1,4</sup>, P. Lebègue<sup>1,4</sup>, L. Cantrel<sup>3,4</sup>, F. Cousin<sup>3,4</sup>, I. Černušák<sup>2</sup>, F. Louis<sup>1,4</sup> (1 Univ. of Lille 1, CNRS, France; 2 Department of Physical and Theoretical Chemistry, Slovakia; 3 Institut de Radioprotection et de Sureté Nucléaire, France; 4 Laboratoire de Recherche Commun IRSN-CNRS-Lille 1, France)

10.20 **Thermal destruction of chemical warfare agents**

J.-C. Lizardo-Huerta<sup>1</sup>, B. Sirjean<sup>1</sup>, L. Verdier<sup>2</sup>, R. Fournet<sup>1</sup>, P.-A. Glaude<sup>1</sup> (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<sup>1,2</sup>, B. Yang<sup>1</sup>, F. Zhang<sup>2</sup> (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

*Chairmen: M. Keller (IFPEN, France) and T. de Bruin (IFPEN, France)*

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 and material properties with the ADF modeling suite

T. M. Soini (Software for Chemistry and 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

*Chairpersons: C. Chizallet (IFPEN, France) and C. Dujardin (Univ. of Lille, France)*

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

**Topical review: challenges in environmental catalysis**

17.00 DFT study of H<sub>2</sub>O and NH<sub>3</sub> coordination capacity at copper in Cu-SSZ-13

B. Kerkeni<sup>1,2</sup>, D. Berthout<sup>1</sup>, D. Berthomieu<sup>3</sup>, C. Chizallet<sup>1</sup> (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<sup>1,2,3</sup>, I. Hitchcock<sup>4</sup>, M. Sarwar<sup>4</sup>, I.P. Silverwood<sup>4</sup>, S. Hindocha<sup>4</sup>, C.R.A. Catlow<sup>1,2</sup>, A.P.E. York<sup>4</sup>, P. J. Collier<sup>2,4</sup>

(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 Pt<sub>13</sub>/γ-Al<sub>2</sub>O<sub>3</sub> clusters

A. Sangnier<sup>1</sup>, C. Chizallet<sup>1</sup>, A. Nicolle<sup>1</sup>, C. Dujardin<sup>2</sup> (1 IFPEN; 2 Univ. of Lille, France)

18.15 Simulation of perovskite materials in emissions control catalysis

C. S. Cooper<sup>1,2</sup>, M. Sarwar<sup>1</sup>, K. Simmance<sup>1</sup>, A.P.E. York<sup>1</sup>, C.R.A. Catlow<sup>2</sup>  
(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

*Chairman: T. de Bruin (IFPEN, France)*

9.00 Plenary Lecture by **William A. Goddard** (Caltech, USA)  
**Advances in multiscale methods for environmentally-friendly design**

9.45 Round Table

*Moderators: C. Chizallet, M. Matrat and T. de Bruin (IFPEN, France)*

Challenges for pollutant mitigation: under-researched areas, human-machine interactions, first-principle/multiscale-based design

Participants: A. Pires Da Cruz (IFPEN, France), L. Rouïl (INERIS, France), M. Sarwar (Johnson Matthey, UK), W. A. Goddard (Caltech, USA), B. Sirjean (Univ. of Lorraine, France) and P. Pullumbi (Air Liquide, France)

11.15 Break and poster session

### SESSION 4: PLASMA CHEMISTRY

*Chairwoman: F. Zhang (Univ. of Science and Technology of China)*

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. Brault<sup>1</sup>, E. C. Neyts<sup>2</sup> (1 GREMI, CNRS Univ. of Orléans, France; 2 Department of Chemistry, Univ. of Antwerp, Belgium)

12.45 Closing remarks  
Theodorus de Bruin, Scientific correspondent of Computational Chemistry conference (IFPEN, France)

12.50 End of the conference

## Poster session

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

S. Pamungkas<sup>1</sup>, N. J. Trilaksono<sup>1</sup> (1 Weather and Climate Prediction Lab., Indonesia)

### Interaction of ozone with KI aerosols

F. Allouti<sup>1,4</sup>, S. Souvi<sup>2,4</sup>, A. Markovits<sup>3</sup>, F. Louis<sup>1,4</sup> (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 C<sub>6</sub>H<sub>5</sub>+C<sub>2</sub>H<sub>2</sub> 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. Dementieva<sup>1</sup>, E. B. Markova<sup>1,2</sup> (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)

### How oxygen vacancies activate CO<sub>2</sub> dissociation on TiO<sub>2</sub> anatase (001)

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

### The surface chemistry of methane 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<sup>1,2</sup>, A. Efendi<sup>1</sup>, E. Babayev<sup>1</sup> (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. Cherqui<sup>1</sup>, A. R. Yeddou<sup>1,2</sup>, F. Halet<sup>1,2</sup>, A. Chergui<sup>1,3</sup>, B. Nadjemi<sup>1</sup>, A. Oulddris<sup>4</sup> (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. Sabour<sup>1</sup>, C. Especel<sup>2</sup>, C. Fontaine<sup>2</sup>, M. Bidaoui<sup>3</sup>, L. Benatallah<sup>1</sup>, N. Bouchenafa-Saib<sup>1</sup>, J. Barbier Jr<sup>2</sup>, O. Mohammedi<sup>1</sup> (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 CO<sub>2</sub> adsorption on the activated carbon: role of disordered network, size effect and temperature

D. Nguemalieu Kouetcha<sup>1</sup>, H. Ramézani<sup>2</sup>, N. Cohaut<sup>1</sup> (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. Jedidi<sup>1</sup>, A. H. Al-ShaikhAli<sup>2</sup>, Dalaver H. Anjum<sup>2</sup>, L. Cavallo<sup>2</sup>, K. Takanebe<sup>2</sup> (1 King Abdulaziz Univ.; 2 King Abdullah Univ. of Science and Technology, Saudi Arabia)

Generation of soot basal structure units with ReaxFF

M. Keller<sup>1</sup>, T. de Bruin<sup>1</sup>, A. Nicolle<sup>2</sup> (1 IFPEN; 2 Paris-Saclay Univ. / ENSTA Paris Tech, France)

*With the support of:*



**SCIENOMICS**  
delivering science



#Compchem2017



*Under the auspices of:*

