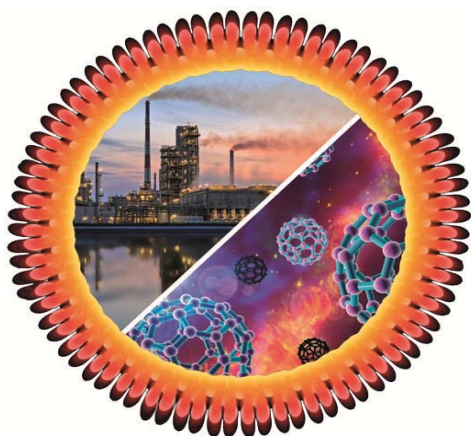


Round table discussion

(Tuesday, March 14th 2017)



Dr. Robin Chaudret (Scienomics)
Prof. William A. Goddard III (Caltech)
Dr. Antonio Pirez Da Cruz (IFPEN)
Dr. Pluton Pullumbi (Air Liquide)
Dr. Misbah Sarwar (Johnson Matthey)
Dr. Baptiste Sirjean (CNRS, Univ. Lorraine)
Prof. Angela Violi (University Michigan)



SCIENOMICS
delivering science



Dr. Robin Chaudret

● Lead Scientist Materials Simulations (Scienomics)

- *Master, Université Pierre et Marie Curie (Paris VI (Paris VI), 2008;*
- *Diplome de l'Ecole normale supérieure 2009;*
- *Ph.D. Université Pierre et Marie Curie, 2011;*
- *Postdoc Duke University, Durham, USA, 2011-2012;*
- *Postdoc IFP Energies nouvelles, 2012-2013;*
- *Scienomics, Research Scientist 2013-2016;*

● Current research interests:

- *Field of expertise;*
- *Research group*
- *Scientific projects;*
- *Collaborations;*
- *Long term scientific objectives;*
- *...*



Prof. William A. Goddard III

● Charles and Mary Ferkel Professor of Chemistry, Materials Science, and Applied Physics

- *B.S., University of California (Los Angeles), 1960;*
- *Ph.D., Caltech, 1965.*
- *Noyes Research Fellow in Chemistry, 1964-66;*
- *Noyes Research Instructor, 1966-67;*
- *Assistant Professor of Theoretical Chemistry, 1967-71;*
- *Associate Professor, 1971-74;*
- *Professor, 1974-78;*
- *Professor of Chemistry and Applied Physics, 1978-84;*
- *Ferkel Professor of Chemistry, 1984-2001;*

● Current research interests:

- Biotechnology
- Polymers
- Catalysis
- Semi-conductors
- Ceramics
- Metal alloys
- Nanoscale systems
- Environmental



Dr. António Pires da Cruz

● Section Head Automotive Engine and Vehicle Modeling at IFP Energies nouvelles

- *Mechanical Engineer in Fluid mechanics and Thermodynamics , Lisbonne (Portugal) 1993;*
- *Ph.D. Université Pierre et Marie Curie (Paris VI), Turbulent combustion, 1997;*
- *Postdoc at ExxonMobil 1998-2000;*
- *IFP-School: Associate Professor 2000-2004*
- *IFP Energies Nouvelles 2004-now;*
- *HDR Institut National Polytechnique of Toulouse, Combustion, CFD, Internal Combustion Engines 2012.*



● Current research interests:

- *Field of expertise: CFD Turbulent Combustion Modeling and Simulation;*
- *Research Group: 20 Engine and Vehicle modeling engineers, 10 PhD Students*
- *Scientific projects: Modeling of turbulence / chemistry interactions for internal combustion engine applications;*
- *Collaborations: Auto and Oil OEMs, Universities (France and Europe), US National Labs;*
- *Long term scientific objectives: Popularize engine and vehicle simulation in a very likely future widespread Connected Mobility context;*

Dr. Pluton Pullumbi

● International Fellow Air Liquide

- *Master University of Tirana (Albania) 1986;*
- *Assistant Professor of Physical Chemistry, University of Tirana 1987-1990;*
- *Ph.D. Université Pierre et Marie Curie (Paris VI) Molecular Spectroscopy, Computational Chemistry, 1994;*
- *Researcher CNRS LIMSAG Laboratory (Dijon, France) 1994-1996;*
- *R&D engineer Air Liquide, 1996 -2000;*
- *Expert Air Liquide, 2000- 2009;*
- *Senior Expert R&D, Air Liquide 2009-2015;*



● Current research interests:

- *Field of expertise; Computational Chemistry-reactivity, Molecular simulations applied to adsorption/permeation, gas separation technology, multi-objective optimization*
- *Scientific projects; Materials discovery for Air Liquide internal applications (Gas separation/storage, catalysis, semiconductors, Healthcare, life-sciences) Process simulation (gas separation by adsorption/permeation)*
- *Collaborations; Several academic groups, research organizations and industrial partners*
- *Long term scientific objectives; Extensive use of computational chemistry to generate data for internal use*

Dr. Misbah Sarwar

● Principal Scientist at Johnson Matthey

- MSci Chemistry University College London, 2002;
- Ph.D. Royal Institution of Great Britain/UCL, 2006;
- Research Scientist Johnson Matthey 2007 – Fuel Cells;
- Senior Scientist Johnson Matthey 2010 – Core Science;
- Principal Scientist Johnson Matthey 2013 – Emissions Control Research;



● Current research interests:

- *Field of expertise; Computational Chemistry, DFT, QM/MM, Molecular Dynamics;*
- *Research group; Part of a team of 8 Scientists based in the UK and South Africa;*
- *Scientific projects; Zeolites for deNOx applications, Novel catalysts for Fuel Cells, Computational Chemistry and characterisation*
- *Collaborations; UCL, Southampton, Oxford, Cambridge*
- *Long term scientific objectives; Linking length and time-scales, Correlating computational chemistry and experimental results*
- ...

Dr. Baptiste Sirjean

● Researcher at CNRS, Laboratoire Réactions et Génie des Procédés University of Lorraine

- *Master, Université Henri Poincaré, Nancy, 2004*
- *PhD, Institut National Polytechnique de Lorraine, Nancy, 2007*
- *Postdoc, University of Southern California (Los Angeles), 2007 – 2009*
- *CNRS Research Scientist, LRGP, Nancy, 2009 -*



● Current research interests:

- *Combustion chemistry; Theoretical chemistry; Chemical Kinetics; Liquid phase oxidation; Thermal destruction of toxics; Automatic generation of kinetic models*
- *Chemical Reactions and Process Engineering Laboratory; Kinetics, Thermodynamic, Energy research axis*
- *Thermal decomposition of chemical warfare (DGA); Combustion kinetics for gas turbine applications (GE Energy Product – Europe); Sulfur Sequestration (Carnot); Kinetic modeling of hydrocarbons autoxidation (MENSUR); Smart additives for variable RON fuels development (SINTEF - MAN);*

Prof. Angela Violi

- Professor of Mechanical Engineering, Chemical Engineering
- Professor of Macromolecular Science and Engineering, & Biophysics
 - *Ph.D. in chemical engineering University of Naples Federico II*
 - *Associate professor 2006-2015*



● *Current research interests:*

- Multiscale simulations of complex systems:
 - nanoparticle growth and self-assembly,
 - nanoparticle interactions with biomolecular systems,
- Applied chemical kinetics
- Aerosols
- Chemical and physical properties of fuels, alternative fuels, lubricants.

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