



SYMPOSIUM IN HONOR OF HERVÉ TOULHOAT

"Rational Approaches to
Catalysts and Materials
for Energy"

PARIS

June 19 & 20


June 19, 2018

PROGRAM

- 13:30 **OPENING**
Sorbonne Université
- 14:00 **J.-C. PLUMAIL & P. SARRAZIN - AXENS**
"Contribution of Hervé Toulhoat to the industrial development of hydrotreating catalysts"
- 14:20 **P. DUFRESNE - EURECAT**
"Some of Eurecat innovations since the mid-eighties (one with Hervé contribution)"
- 14:50 **B. SILVI - EMERITUS SORBONNE UNIVERSITÉ (SU)**
"Electron localization function and Lewis's heritage: chemical interpretation in quantum chemistry"
- 15:20 **M. MARSMAN - UNIVERSITY OF VIENNA**
"VASP: past, present, future"
- 15:50 **R. VAN SANTEN - EINDHOVEN UNIVERSITY OF TECHNOLOGY**
"Mechanism of the Fischer-Tropsch reaction"
- 16:20 
- 17:00 **A. FUCHS - PSL UNIVERSITY**
"Hervé Toulhoat and the issue of molecular chemistry software"
- 17:20 **P.-H. BIGEARD - IFPEN**
"Hervé Toulhoat : his contributions at IFP Energies nouvelles"
- 17:40 **K. REUTER - TECHNICAL UNIVERSITY OF MUNICH**
"A look through the operando glass: First-principles multiscale modeling of working catalysts"
- 18:10 **E. WIMMER - MATERIALS DESIGN**
"Art in Computational Materials Science"

June 20, 2018

PROGRAM

- 09:00 **P. RAYBAUD - IFPEN**
"Computational design of transition metal sulfides: a volcano of inspiration"
- 09:30 **M. BREYSSE & C. GEANTET - FORMERLY SU & IRECELYON**
"From the characterization of industrial and model catalysts to the rational approach of new phases and supports: 20 years of collaboration with Hervé"
- 10:00 **E. PAYEN - EMERITUS UNIVERSITY OF LILLE**
"From the HDS/HDT catalysts synthesis to the active phases modelling: A brief history of the relations of Hervé Toulhoat with the Lille Laboratory of Catalysis"
- 10:30 
- 11:00 **R. PRINS - EMERITUS ETH ZURICH**
"What can we learn from gamma-iron/gallia oxides to understand the structure of gamma-alumina?"
- 11:30 **B. SMIT - EPFL LAUSANNE**
"The Nanoporous Materials Genome in Action"
- 12:00 **M. CHE - EMERITUS SU**
"Thirty years already! a collaboration between IFP/IFPEN and UPMC/Sorbonne-Université experienced by two friends"



Acknowledgments & Closing



HERVÉ TOULHOAT



Dr. Hervé Toulhoat, born april 1954, received his Chemical Engineering degree from the Paris School of Chemistry (now Chimie Paristech) in 1976, then went on to earn his PhD from the Paris School of Mines (Mines Paristech) in 1980. In 2002, Dr. Toulhoat received his Habilitation from University Pierre et Marie Curie (now Sorbonne Université).

Dr. Toulhoat was the Deputy Scientific Director of IFP Energies nouvelles (IFPEN) until his retirement (December 31st, 2016). Since joining IFP in 1980, Dr. Toulhoat has served numerous positions, including: research Scientist, then Project Manager "Basic and Exploratory Research in Hydrotreatments", Division Kinetics and Catalysis, (1980-1987); head of the Department of Physical Chemistry of Interfaces (1987-1992); in charge of the Molecular Modelling Group, Division of Computer Science and Applied Mathematics (1995-2000); director of the "European GdR" CNRS G12090 "Dynamique moléculaire quantique appliquée à la catalyse, l'adsorption et l'absorption" (1996-2003); IFP Associate Research Director (1998-2005); director of Doctoral Studies at IFP School (2001-2012); In charge of IFPEN exploratory research (May 1998-2016).

Dr. Toulhoat also spent time at Total Raffinage Distribution (1993-1994) as a Scientific Consultant, in charge of developing molecular modelling.

His teaching activities have included: organization of IFP School Doctoral College Conferences (2001-2012); lectures on molecular modelling for various Masters of Science (Paris, Marne la Vallée, Lyon) (1995-present) and at IFP School on hydrotreating catalysts and processes (1982-1987).

Dr. Toulhoat's current research topics are applications of molecular modelling and computational chemistry in catalysis, while his fields of competence include Catalysis, Chemistry, Physical Chemistry of Surfaces and Interfaces, Chemical Engineering, Refining and Petrochemistry, Molecular Modelling, and Theoretical Chemistry.

In addition to serving on the Editorial Board of "Journal of Catalysis" since 2005, Dr. Toulhoat is also a member of the Editorial Board of l'Actualité Chimique, a member of the Société Chimique de France, active in the board of the "interdivision énergie", and a member of the executive scientific committee of IUPAC 2019.

Dr. Toulhoat has authored or co-authored 133 publications, and 24 patents, has directed 14 doctoral theses, and coordinated 7 books or proceedings. He has been invited several times as keynote speaker to international conferences : EUROPACAT VIII, FOMMS 2009, CIMAT 2008, MIGRATION 05, OXYSOL 2005, NCCC VII, etc... He has organized or co-organized several international workshops. He has been promoter and coordinator of 5 international or national large collaborative projects and active member of 2 more.

Dr. Toulhoat has also been the recipient of a number of awards, including the following: Chevalier de l'Ordre National du Mérite (2005), Prix Michonsniky of Chimie Paristech alumni (1988), and Silver Medal, "Société pour l'Encouragement de l'Industrie Nationale" (1985).

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