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Keywords

Physical adsorption of gases and liquids Characterization of porous solids Adsorption and immersion calorimetry Thermal Analysis of powders and adsorbents

Research interests

Gas adsorption : special attention to its thermodynamic study in view of characterizing either the adsorption mechanism and the state (structure, mobility) of the adsorbed phase or the porous structure of the adsorbent. Special interest for the determination of the surface area of adsorbents. Introduction and generalization of quasi-equilibrium procedures, in either adsorption gravimetry (the first on-line, continuous recording of a gas adsorption-desorption isotherm), adsorption manometry and microcalorimetry (after developing what is to-day the only experiment able to directly measure the differential enthalpy of adsorption of a gas at 77 or 87 K). Development, in 2001-2004, of the first experiment allowing to study the co-adsorption of up to 5 gases, up to 50 bar, for the sake of gas separation and storage.

Liquid adsorption : mainly interested by its microcalorimetric study (assessment of enthalpies of immersion, displacement, intrusion ...) and its application to the characterization of solid surfaces (surface area, size of micropores, chemical state of the surface). Development, in 2000-2001, of the novel method of immersion microcalorimetry into liquid argon which, with the help of modelling, was shown to be, a sound way to assess the specific surface area of a microporous oxide (silica-gel, zeolite, activated alumina, magnesia, beryllia, titania, zirconia etc...).

Thermal transformation of powders and nanoporous materials: proposal and development of the novel and general method of Controlled Rate Thermal Analysis (CRTA), which provides enhanced resolution and lends itself to a new approach to kinetics (with the "rate-jump" method for an assumption-free determination of the energy of activation). Application to the preparation of technological adsorbents with tailor-made porosity and highly reproducible surface properties. In the nineties, this approach was generalized under the generic and well-accepted name of Sample-Controlled Thermal Analysis (SCTA).

30th March 2022



Background

1964: Gets his "Doctorat d'Etat ès-Sciences Physiques" in the Sorbonne, Paris, on the « Thermal preparation and transformation of porous alumina, beryllia, and silica-alumina ». 1966: Enters the staff of the CNRS (Centre National de la Recherche Scientifique) in the "Thermodynamics and Microcalorimetry Center" in Marseille and then launches a research group on the « Thermoanalytical and thermodynamic study of technological adsorbents ».

1972: "Directeur de Recherches" in the CNRS

2002 : "Directeur de Recherches Emérite" in MADIREL, a joint laboratory between CNRS and Aix-Marseille University.

Past and current commitments

- Director, from 1990 to 2002, of the "CNRS Thermodynamics and Microcalorimetry Center" in Marseille (founded by Prof. E.Calvet in 1959 and then the "cradle" of heatflowmeter microcalorimetry) and Deputy-Director from 1975 to 1989)
- Chairman of Commission I-6 (Colloid and Surface Chemistry including Catalysis) of IUPAC (International Union of Pure and Applied Chemistry), from 1991 to 1994
- Chairman of the IUPAC Sub-Committee on the Characterization of Porous Solids, from 1985 to 1994
- Chairman of the IUPAC Task-Group on "Liquid intrusion and alternative methods for the characterization of macroporous solids" for the period 2006-2012
- Member of the IUPAC Task-Group on "Physisorption of gases, with special reference to the evaluation of surface area and pore-size distribution" for the period 2011-2015
- President (2000-2006) of ICTAC, the International Confederation of Thermal Analysis and Calorimetry, which federates 23 National Associations and gathers ca 5000 scientists
- President of the French Association for Calorimetry and Thermal Analysis (AFCAT), from 1985 to 1989
- President of "Eurosolid" (European Association on the Reactivity of Solids), from 1997 to 2001
- Member of the Editorial or Advisory Board of Journals dealing with either Thermal Analysis (« Thermochimica Acta », 1989-2004, « Journal of Thermal Analysis and Calorimetry », from 2007) or Adsorption (« Adsorption Science and Technology », 1984-1995, « Colloid and Interface Science », 1982-1985, « Chemical Technology and Biotechnology »,1978-1986, « Langmuir », 1985-1988, and « Adsorption », 1993-2013.

Scientific production

ca. 200 published papers, 100 invited lectures in international conferences, 150 oral presentations in conferences or lectures in universities and laboratories and 8 books (editor or author). The following gives an idea of their principal orientations:

The book « Adsorption by powders and porous solids: principles, methodology and applications »

1st edition: ROUQUEROL F., ROUQUEROL J. and SING K.S.W.

Academic Press, 1999, 467 pages. 2nd edition: ROUQUEROL F., ROUQUEROL J., SING K.S.W., P.LLEWELLYN and G.MAURIN Academic Press, 2014, 626 pages.

The IUPAC Report on « Liquid intrusion and alternative methods for the characterization of macroporous materials »

ROUQUEROL J., BARON G., DENOYEL R., GIESCHE H., GROEN J., KLOBES P., LEVITZ P., NEIMARK A., RIGBY S., SKUDAS R., SING K.S.W., THOMMES M., UNGER K.K. Pure Appl. Chem. 2012, Vol 84, n⁰1, 107-136.

The IUPAC Report "Physisorption of gases, with special reference to the evaluation of surface area and pore size distribution"

THOMMES M., KANEKO K., NEIMARK A.V., OLIVIER J.P., RODRIGUEZ-REINOSO F., ROUQUEROL J., SING K.S.W (IUPAC Technical Report), Pure & Appl. Chem. 87 (9-10), 1051-1069 (2015)

The chapter "Principles and Applications of Calorimetry"

In: REEDIJK, J. (Ed.) ROUQUEROL J., ROUQUEROL F., LLEWELLYN P., DENOYEL R., Elsevier Reference Module in Chemistry, Molecular Sciences and Chemical Engineering. Waltham, MA: Elsevier. 27-May-2015 <u>http://dx.doi:10.1016/B978-0-12-409547-2.11009-1</u>

The book « Sample-Controlled Thermal Analysis: origin, goals, multiple forms, applications and future $\, \gg$

SORENSEN O.T. and ROUQUEROL J. Eds. Kluwer Academic Publishers, Dordrecht, Boston, London, 2003, 252 pages

The chapter « **Developments in Nomenclature in Thermal Analysis and Calorimetry**» ROUQUEROL J., WADSO I., LEVER T.J. and HAINES P.J. Chapter 2 In "Handbook of Thermal Analysis and Calorimetry", Volume 5, "Further Advances,

Techniques and Applications", M.Brown and P.Gallagher Eds, Elsevier, Amsterdam, 2007, pp 13-54

The chapter "**Thermal Analysis : Sample-Controlled Techniques**" ROUQUEROL J.

In: Encyclopedia of Analytical Science (3rd Ed.), Worsfold, P., Poole, C., Townshend, A., Miró, M., (Eds.), Elsevier, 2019, vol 10, pp 17-32

Awards

-Bronze (1966) and Silver (1971) medal of the French Society for National Industry

-Bronze medal of the Centre National de la Recherche Scientifique (CNRS) (1971)

-Lucien Chatin Award of Lyon Academy (1972)

-Mettler Award of the North American Thermal Analysis Society (NATAS) (1988)

-Doctor Honoris Causa of UNED University, Madrid, Spain (2003)

-Provence award of the Société Chimique de France (2013)

-AICAT-Setaram Award of the Italian Association of Calorimetry and Thermal Analysis (2013)

-STK Award of the Swiss Association of Calorimetry and Thermal Analysis (2018)

-ICTAC Distinguished Service Award (2016) and Robert Mackenzie Lectureship (2021) of the International Confederation of Thermal Analysis and Calorimetry

-Edouard Calvet Award of the French Association of Calorimetry and Thermal Analysis (2022)