SEMINAR

October 19th, 2017

IMDEA Energy, in collaboration with Instrumentación Específica de Materiales, IESMAT, organizes a one day event:

CHARACTERIZATION OF NANOPOROUS MATERIALS: RECENT ADVANCES

VENUE: IMDEA ENERGY - Avenida Ramón de la Sagra, 3 – Parque Tecnológico de Móstoles – 28935 - Móstoles (Madrid)

DATE: Thursday October 19th 2017, starting at 09:00 AM.

With the collaboration of:

REGISTRATION: Registration fee € **50 (IVA/VAT included)**, In order to attend you must send an email to Estefania.ecija@iesmat.com with a document showing the bank transfer to the account INSTRUMENTACION ESPECIFICA DE MATERIALES, S.A. - Banco Sabadell-Atlántico - 0081-0299-91-0001290536**. All attendees must include the DNI or passport number in order to access the Venue. Please make sure to register before October 13th.**

All conferences will be in English language without translation

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PROGRAMME

9:00-9:30 – Registration

9:30-9:35 – **Welcome address** (David Serrano – IMDEA Energy, David Grela – IESMAT)

9:35-10:15 - **High Pressure and Competitive Gas Adsorption for Characterizing Solids for Gas Storage and Separation** (Charles Thibault – Quantachrome Instruments)

10:15-11:15 - Probing the porosity of hierarchical zeolites by gas adsorption techniques (David Serrano – IMDEA Energy)

11:15-11:45 - **Coffee break**

11:45-12:30 - Vapor and Reactive Gas Adsorption for Characterizing Solids Regarding Surface Chemistry and Catalysis (Charles Thibault – Quantachrome Instruments)

12:30-13:30 - Gas/vapour adsorption combined with immersion calorimetry as a powerful tool for the characterization of porous solids (Joaquin Silvestre Albero – University of Alicante)

13:30-14:30 – Lunch

14:30-15:30 – **Application of zeolites in adsorption and separation processes** (Eduardo Pérez-Botella, Miguel Palomino, Susana Valencia, Fernando Rey - Instituto de Tecnología Química, Universitat Politècnica de València-Consejo Superior de Investigaciones Científicas, Valencia, Spain)

15:30 -16:30 - **Recent Advances in the Textural Characterization of Hierarchically Structured Nanoporous Materials** (Matthias Thommes – Quantachrome Instruments)

16:30 – Closure

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ABSTRACTS

High Pressure and Competitive Gas Adsorption for Characterizing Solids for Gas Storage and Separation

Charles Thibault
Quantachrome Instruments , Boynton Beach, Fl 33426 ,USA

Abstract

Use of adsorbents, both naturally occurring and synthetic, for the capture and storage of gasses has been of interest for many years. Removal of CO_2 and other greenhouse gasses from industrial effluent is an important process for reducing the amount of these greenhouse gasses released into the atmosphere. Storage of CO_2 for use in subsequent processes or for sequestration is just as important as its removal. Storage of H_2 and CH_4, among other gasses is important in the transport and use of alternative fuels. Removal of CO_2 from CH_4 or H_2 is another application where adsorbents play a critical role. Dynamic high-pressure gas sorption is a valuable tool for characterizing not only the capacity, but also the competitive adsorption of gasses on an adsorbent used for gas separation and purification. This seminar discusses some recent works in these areas, where both static and dynamic high-pressure gas sorption was used for the characterization and evaluation of these adsorbents.

Probing the porosity of hierarchical zeolites by gas adsorption techniques

David P. Serrano
IMDEA Energy, Rey Juan Carlos University

Summary

Hierarchical zeolites have arisen high interest in the last years since the presence of a secondary porosity in these materials, located usually in the mesopore range, provides a number of relevant advantages compared to conventional zeolites. Thus, hierarchical zeolites show lower steric and diffusional constraints when processing large molecules, whereas the deactivating effects of coke deposition are less pronounced. Moreover, the secondary porosity represents an ideal space for the deposition of other active phases (mainly metals and metal oxides) with high dispersion over the support, leading to materials with remarkable performance as bifunctional catalysts. As a consequence, hierarchical zeolites have expanded the number and variety of catalytic applications typical of zeolitic materials.

Determination of the textural properties of hierarchical zeolites is not a straightforward task due to the simultaneous presence of different levels of porosities: micropores, mesopores an interstitial porosity. Among the different techniques and methods available, NL-DFT models applied to the Ar adsorption isotherms have proved to be reliable and very useful approaches for characterizing the porosity of hierarchical zeolites, allowing the determination of a variety of properties, such as the pore size distribution, surface areas and pore volumes corresponding to both micro- and mesopores.

Vapor and Reactive Gas Adsorption for Characterizing Solids Regarding Surface Chemistry and Catalysis

Charles Thibault
Quantachrome Instruments , Boynton Beach, Fl 33426 ,USA

Abstract

Solid-gas reactions occur at the surface of the solid, where the solid and the gas interact. Whether the solid acts as a catalyst in the reaction of the gasses or is a reactant itself, it is important to understand the nature of the surface. BET surface area is a critical characteristic in determining the reactivity of the solid, but the surface chemistry, including its affinity to the vapors or gasses being reacted, is just as important. Both static vapor sorption and dynamic chemisorption provide valuable information in this regard. This seminar discusses the techniques used in this characterization.

Gas/vapour adsorption combined with immersion calorimetry as a powerful tool for the characterization of porous solids

Joaquín Silvestre Albero
Inorganic Chemistry Dept. University of Alicante

Summary

The knowledge of the textural properties when dealing with nanoporous solids is of paramount important to understand their performance in a given application. N_2 adsorption at 77K has been traditionally applied for the determination of the main textural parameters, for instance BET surface area, micropore volume and total pore volume. However, the low temperature of the measurement and the associated quadrupole moment could give rise to erroneous determination of the adsorption isotherm, when dealing with samples with narrow constrictions or with a rich surface chemistry. In this sense, the application of other probe molecules (e.g. Ar at 87 K or CO2 at 273 K) can be very useful to overcome some of

these limitations. Although this is straightforward for carbon materials, this is not the case for certain MOFs where the presence of structural phenomena (e.g. breathing phenomena) has to be considered.

Immersion calorimetry into liquids of different molecular dimensions (dichloromethane, benzene, 2,2-dimethyl butane, α-pinene, etc.) is a powerful and easy technique for the characterization of the microporosity (surface area and pore size distribution) in activated carbons. In this sense, for solids with a similar surface chemistry, as in the case of activated carbons and carbon molecular sieves, i.e. in the absence of specific interactions between the solid surface and the immersion liquid, the heat of immersion has been shown to be proportional to the surface area available for the specific liquid. Consequently, immersion calorimetry can be considered as a valuable technique to complement gas adsorption for the characterization of carbon materials. However, as described above, this is not that easy in the case of MOFs due to the presence of specific interactions, for instance with exposed metal centres.

Application of zeolites in adsorption and separation processes

Eduardo Pérez-Botella, Miguel Palomino, Susana Valencia, Fernando Rey
Instituto de Tecnología Química, Universitat Politècnica de València-Consejo Superior de Investigaciones Científicas, Valencia, Spain

Zeolites are microporous solids that possess structural channels and cavities of molecular dimensions as well as high adsorption capacities. These properties confer them extraordinary potential application for molecular separation processes. However, the selection of the most appropriate zeolite as adsorbent for a particular separation can be rationalized in terms of pore aperture, channel system dimensionality and polarity. Examples of the tuning of these properties for target separations will be explained aiming to illustrate the strategies pursued for achieving successful separations.

Recent Advances in the Textural Characterization of Hierarchically Structured Nanoporous Materials

Matthias Thommes
Quantachrome Instruments , Boynton Beach, Fl 33426 ,USA

Abstract

In recent years, major synthetic efforts have been focused on the introduction of hierarchical pore structures into many different materials such as zeolites, carbons, silicas, MOFs, hybrid layered and pillared structures. Nanoporous materials which consist of

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hierarchical pore networks with pore widths spanning the entire micro-mesopore range (i.e. up to 50 nm) allow one to overcome accessibility and diffusion limitations associated with classical microporous materials for catalysis and separations.
In this talk, recent developments in the structural characterization of these materials will be described. An accurate textural characterization is crucial not only within the discovery process of novel hierarchically ordered nanoporous materials but also contributes to advance their application in a variety of areas including heterogenous catalysis, separation, battery devices, drug delivery. Among a variety of techniques, gas adsorption is widely applied because it assesses a wide range of pore sizes, spanning the entire micro- and mesopore range. Within the last two decades major progress has been achieved in physical adsorption characterization also because of the development of advanced approaches based on statistical mechanics such as molecular simulation and density functional theory (DFT) [1]. This progress, coupled with the availability of high resolution experimental methodologies for the adsorption of various subcritical fluids (also allowing one to couple adsorption techniques with complimentary techniques such as small angle scattering), has led to major advances in the structural characterization of nanoporous materials. However, major challenges still exist concerning an in-*depth* characterization of complex pore networks. Application of characterization techniques to hierarchical materials has revealed new phenomena, such as cavitation processes during desorption, and led to significant refinement of these techniques [2]

[1] M. Thommes, K. Kaneko, A.V. Neimark, J.P. Olivier, F. Rodriguez Reinoso, J. Rouquerol and K.S.W Sing, (IUPAC Technical Report), *Pure Appl. Chem.* **87**, 1051 (2015)
[2] K. A. Cychosz, R. Guillet-Nicolas, J. Garcia-Martinez, J., M. Thommes, M. *Chem. Soc. Rev.* **46**, 389, (2017)

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