

New and improved models for the enhanced characterization of porous materials such as carbons, zeolites, and MOFs

Micromeritics' ongoing commitment to NLDFT models for greater accuracy in porosity characterization

NORCROSS, GEORGIA, UNITED STATES, May 19, 2020 /EINPresswire.com/ -- Micromeritics Instrument Corp., a global leader in material characterization technologies, offers a number of non-local density functional theory (NLDFT) models which underlines its ongoing commitment to refine the performance of gas adsorption techniques for materials with microporous structure. Customers can pick from more than 30 NLDFT models to match the properties of their material (chemical composition, pore geometry) and understand pore size distribution of a probe more effectively. The company also offers what is believed to be the first commercially available NLDFT model for a MOF (metal organic framework). Micromeritics customers can download any of the models, free of charge, and have access to future models as they are developed and released.

Easily applied with existing software, the models improve the accuracy of [porosity](#) metrics derived from gas adsorption data: Porosity is performance-defining for many materials, with pore structure at the micropore scale (<2nm) increasingly of interest for industrial applications. Gas adsorption is a well-established technique for porosity characterization, but its application becomes more challenging in the microporous region. NLDFT, which involves molecular modelling, generates accurate values of the physical properties of an adsorptive, notably density, inside pores, where fluid behavior is modified by interactions with pore walls. Relevant NLDFT models therefore play a crucial role in the conversion of measured gas adsorption isotherms into precise and accurate porosity data.

Micromeritics have long pioneered the application of NLDFT models and offer software which



WHITEPAPER

AN INTRODUCTION TO NLDFT MODELS
FOR POROSITY CHARACTERIZATION

Micromeritics' whitepaper introducing
NLDFT models for porosity
characterization

streamlines their efficient application in routine analyses. An ongoing and significant investment in NLDFT modelling is part of the company's commitment to providing access to the very best porosity characterization technology. Available models for example allow customers to:

- Extend the use of argon (Ar) as a sorptive for carbons and zeolites (oxides) to address well-documented limitations with nitrogen (N₂) for microporous materials.
- Enhance the use of oxygen (O₂) as a sorptive for carbons. For micropore analysis O₂ is a less expensive alternative to Ar with superior performance to N₂.
- Begin to apply NLDFT modelling to MOFs, a complicated process due to their diverse chemistry.



For an introduction to NLDFT, and its importance, Micromeritics has collected frequently answered questions on this complex topic in an easy-to-understand whitepaper that can be downloaded at micromeritics.com/NLDFT.

About Micromeritics Instrument Corporation

Micromeritics Instrument Corporation is a global provider of solutions for material characterization with best-in-class instrumentation and application expertise in five core areas: density; surface area and porosity; particle size and shape; powder flow and bulk characterization; and catalyst characterization and process development. The company is headquartered in Norcross, Georgia, USA and has more than 400 employees worldwide. With a fully integrated operation that extends from a world class scientific knowledge base through to in-house manufacture, Micromeritics delivers an extensive range of high-performance products for oil processing, petrochemicals and catalysts, to food and pharmaceuticals, and works at the forefront of characterization technology for next generation materials such as graphene, metal-organic-frameworks, nanocatalysts, and zeolites.

For additional information visit micromeritics.com

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