Confined benzene within InOF-1: Contrasting CO\textsubscript{2} and SO\textsubscript{2} capture behaviours

Barrios-Vargas, L.J.\textsuperscript{a}  
Ruiz-Montoya, J.G.\textsuperscript{b}  
Landeros-Rivera, B.\textsuperscript{c}  
Álvarez, J.R.\textsuperscript{a}  
Alvarado-Alvarado, D.\textsuperscript{a}  
Vargas, R.\textsuperscript{a}  
Martínez, A.\textsuperscript{d}  
González-Zamora, E.\textsuperscript{e}  
Cáceres, L.M.\textsuperscript{e}  
Morales, J.C.\textsuperscript{b,e}  
Ibarra, I.A.\textsuperscript{a}

\textsuperscript{a}Laboratorio de Fisicoquímica y Reactividad de Superficies (LaFReS), Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Circuito Exterior s/n, CU Coyoacán Ciudad de México, 04510, Mexico  
\textsuperscript{b}Laboratorio de Investigación de Electroquímica Aplicada, Facultad de Ciencias, Universidad Nacional de Ingeniería, Av. Tupac Amaru 210, Rímac Lima, Peru  
\textsuperscript{c}Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa, San Rafael Atlixco 185, Col. Vicentina Iztapalapa Ciudad de México, C. P. 09340, Mexico

Abstract

The confinement of small amounts of benzene in InOF-1 (Bz@InOF-1) shows a contradictory behavior in the capture of CO\textsubscript{2} and SO\textsubscript{2}. While the capture of CO\textsubscript{2} is increased 1.6 times, compared to the pristine material, the capture of SO\textsubscript{2} shows a considerable decrease. To elucidate these behaviors, the interactions of CO\textsubscript{2} and SO\textsubscript{2} with Bz@InOF-1 were studied by DFT periodical calculations postulating a plausible explanation: (a) in the case of benzene and CO\textsubscript{2}, these molecules do not compete for the preferential adsorption sites within InOF-1, providing a cooperative CO\textsubscript{2} capture enhancement and (b) benzene and SO\textsubscript{2} strongly compete for these preferential adsorption sites inside the MOF material, reducing the total SO\textsubscript{2} capture. This journal is © The Royal Society of Chemistry.

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Vargas, R.; Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa, San Rafael Atlixco 185, Col. Vicentina Iztapalapa Ciudad de México, Mexico; email: ruvf@xanum.uam.mx
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