



Document details

1 of 1

[Export](#) [Download](#) [Print](#) [E-mail](#) [Save to PDF](#) [Add to List](#) [More... >](#)[View at Publisher](#)

Dalton Transactions

Volume 49, Issue 9, 7 March 2020, Pages 2786-2793

Confined benzene within InOF-1: Contrasting CO₂ and SO₂ capture behaviours (Article)

Barrios-Vargas, L.J.^a, Ruiz-Montoya, J.G.^b ✉, Landeros-Rivera, B.^c, Álvarez, J.R.^a, Alvarado-Alvarado, D.^a, Vargas, R.^c ✉, Martínez, A.^d, González-Zamora, E.^c, Cáceres, L.M.^e, Morales, J.C.^{b,e} ✉, Ibarra, I.A.^a 👤^aLaboratorio de Fisicoquímica y Reactividad de Superficies (LaFRoS), Instituto de Investigaciones en Materiales,

Universidad Nacional Autónoma de México, Circuito Exterior s/n, CU Coyoacán Ciudad de México, 04510, Mexico

^bLaboratorio de Investigación de Electroquímica Aplicada, Facultad de Ciencias, Universidad Nacional de Ingeniería, Av. Tupac Amaru 210, Rímac Lima, Peru^cDepartamento de Química, Universidad Autónoma Metropolitana-Iztapalapa, San Rafael Atlixco 185, Col. Vicentina Iztapalapa Ciudad de México, C. P. 09340, Mexico[View additional affiliations](#) ▾

Abstract

[View references \(48\)](#)

The confinement of small amounts of benzene in InOF-1 (Bz@InOF-1) shows a contradictory behavior in the capture of CO₂ and SO₂. While the capture of CO₂ is increased 1.6 times, compared to the pristine material, the capture of SO₂ shows a considerable decrease. To elucidate these behaviors, the interactions of CO₂ and SO₂ with Bz@InOF-1 were studied by DFT periodical calculations postulating a plausible explanation: (a) in the case of benzene and CO₂, these molecules do not compete for the preferential adsorption sites within InOF-1, providing a cooperative CO₂ capture enhancement and (b) benzene and SO₂ strongly compete for these preferential adsorption sites inside the MOF material, reducing the total SO₂ capture. This journal is © The Royal Society of Chemistry.

Funding details

Funding sponsor	Funding number	Acronym
Universidad Nacional de Ingenierias		UNI
Instituto de Ciencias Matemáticas		ICMAT
Consejo Nacional de Ciencia y Tecnología	IN101517,236879,1789	CONACYT
Universidad Autónoma Metropolitana		UAM

Funding text

The authors thank Dr A. Tejeda-Cruz (powder X-ray; IIM-UNAM), CONACYT (1789), PAPIIT UNAM (IN101517), México for financial support. E. G.-Z. thanks CONACYT (236879), México for financial support. Thanks to U. Winnberg (ITAM) for scientific discussions. B. L.-R. thanks UAM for a postdoctoral fellowship. We thank the Laboratorio de Supercómputo y Visualización en Paralelo at the Universidad Autónoma Metropolitana (UAM) Iztapalapa for access to their computer facilities. We thank the Instituto de Investigación of the Facultad de Ciencias, UNI for the partial research grant.

[Metrics](#) ⓘ [View all metrics >](#)

PlumX Metrics ▾

Usage, Captures, Mentions, Social Media and Citations beyond Scopus.

Cited by 0 documents

Inform me when this document is cited in Scopus:

[Set citation alert >](#)[Set citation feed >](#)

Related documents

Confined toluene within InOF-1: CO₂ capture enhancementGarrido-Olvera, L.P. , Sanchez-Bautista, J.E. , Alvarado-Alvarado, D. (2019) *RSC Advances*CO₂ capture enhancement for InOF-1: confinement of 2-propanolSánchez-Bautista, J.E. , Landeros-Rivera, B. , Jurado-Vázquez, T. (2019) *Dalton Transactions*Water Adsorption Properties of Fe(pz)[Pt(CN)₄] and the Capture of CO₂ and COAlvarado-Alvarado, D. , González-Estefan, J.H. , Flores, J.G. (2020) *Organometallics*[View all related documents based on references](#)[Find more related documents in Scopus based on:](#)[Authors >](#)

ISSN: 14779226

CODEN: DTARA

Source Type: Journal

Original language: English

DOI: 10.1039/c9dt04667d

PubMed ID: 32043501

Document Type: Article

Publisher: Royal Society of Chemistry

All Export Print E-mail Save to PDF Create bibliography

-
- 1 *Carbon Dioxide Levels Hit Record Peak in May*
National Oceanic and Atmospheric Administration (NOAA)
<https://research.noaa.gov/article/ArtMID/587/ArticleID/2461/Carbon-dioxide-levels-hit-record-peak-in-May>
-
- 2 accessed November 2019
-
- 3 *WMO Greenhouse Gas Bulletin (GHG Bulletin) No.*
World Meteorological Organization (WMO), 14
https://library.wmo.int/doc_num.php?explnum_id=5455
-
- 4 accessed November 2019
-
- 5 Kumar, P., Kim, K.-H., Kwon, E.E., Szulejko, J.E.
Metal-organic frameworks for the control and management of air quality: Advances and future direction

(2015) *Journal of Materials Chemistry A*, 4 (2), pp. 345-361. Cited 62 times.
<http://pubs.rsc.org/en/journals/journalissues/ta>
doi: 10.1039/c5ta07068f

View at Publisher
-
- 6 Kaskel, S.
(2016) *The Chemistry of Metal-Organic Frameworks: Synthesis, Characterization, and Applications*. Cited 208 times.
Wiley-VCH, Weinheim
-
- 7 Farrusseng, D.
Metal-Organic Frameworks: Applications from Catalysis to Gas Storage

(2011) *Metal-Organic Frameworks: Applications from Catalysis to Gas Storage*. Cited 367 times.
<http://onlinelibrary.wiley.com/book/10.1002/9783527635856>
ISBN: 978-352732870-3
doi: 10.1002/9783527635856

View at Publisher
-
- 8 (1982) *Review of the National Ambient Air Quality Standards for Sulfur Oxides: Assessment of Scientific and Technical Information*. Cited 21 times.
Environmental Protection Agency,. Report EPA-450/5-82-007. Research Triangle Park, NC: U.S. Environmental Protection Agency, Office of Air Quality and Program Standards, 225 p
-
- 9 Laskin, S., Kuschner, M., Drew, R.T.
Studies in pulmonary carcinogenesis
(1970) *Inhalation Carcinogenesis*, pp. 321-350. Cited 90 times.
AEC Symposium Series 18, ed. M. G. Hanna Jr., Nettesheim and J. R. Gilbert, U.S. Atomic Energy Commission. Division of Technical Information, Oak Ridge
-

- 10 Kampa, M., Castanas, E.
Human health effects of air pollution
(2008) *Environmental Pollution*, 151 (2), pp. 362-367. Cited 1541 times.
doi: 10.1016/j.envpol.2007.06.012
[View at Publisher](#)
-
- 11 Greenberg, N., Carel, R.S., Derazne, E., Bibi, H., Shpriz, M., Tzur, D., Portnov, B.A.
Different effects of long-term exposures to SO₂ and NO₂ air pollutants on asthma severity in young adults
(2016) *Journal of Toxicology and Environmental Health - Part A: Current Issues*, 79 (8), pp. 342-351. Cited 25 times.
<http://www.tandf.co.uk/journals/titles/15287394.asp>
doi: 10.1080/15287394.2016.1153548
[View at Publisher](#)
-
- 12 *Air Quality Guidelines for Particulate Matter, Ozone, Nitrogen Dioxide and Sulfur Dioxide*. Cited 1685 times.
World Health Organisation (WHO)
http://apps.who.int/iris/bitstream/10665/69477/1/WHO_SDE_PHE_OEH_06.02_eng.pdf
-
- 13 accessed November 2019
-
- 14 Furmaniak, S., Terzyk, A.P., Gauden, P.A., Kowalczyk, P., Szymański, G.S.
Influence of activated carbon surface oxygen functionalities on SO₂ physisorption - Simulation and experiment
(2013) *Chemical Physics Letters*, 578, pp. 85-91. Cited 22 times.
doi: 10.1016/j.cplett.2013.05.060
[View at Publisher](#)
-
- 15 Decoste, J.B., Peterson, G.W.
Metal-organic frameworks for air purification of toxic chemicals
(2014) *Chemical Reviews*, 114 (11), pp. 5695-5727. Cited 506 times.
<http://pubs.acs.org/journal/chcreay>
doi: 10.1021/cr4006473
[View at Publisher](#)
-
- 16 Yang, S., Sun, J., Ramirez-Cuesta, A.J., Callear, S.K., David, W.I.F., Anderson, D.P., Newby, R., (...), Schröder, M.
Selectivity and direct visualization of carbon dioxide and sulfur dioxide in a decorated porous host
(2012) *Nature Chemistry*, 4 (11), pp. 887-894. Cited 274 times.
doi: 10.1038/nchem.1457
[View at Publisher](#)
-
- 17 Ho, L.N., Clauzier, S., Schuurman, Y., Farrusseng, D., Coasne, B.
Gas uptake in solvents confined in mesopores: Adsorption versus enhanced solubility
(2013) *Journal of Physical Chemistry Letters*, 4 (14), pp. 2274-2278. Cited 26 times.
doi: 10.1021/jz401143x
[View at Publisher](#)
-



- 18 Rakotovao, V., Ammar, R., Miachon, S., Pera-Titus, M.
Influence of the mesoconfining solid on gas oversolubility in nanoliquids
(2010) *Chemical Physics Letters*, 485 (4-6), pp. 299-303. Cited 23 times.
<http://www.elsevier.com/locate/cplonline>
doi: 10.1016/j.cplett.2009.12.038
View at Publisher
-
- 19 Luzar, A., Bratko, D.
Gas solubility in hydrophobic confinement
(2005) *Journal of Physical Chemistry B*, 109 (47), pp. 22545-22552. Cited 48 times.
doi: 10.1021/jp054545x
View at Publisher
-
- 20 Bratko, D., Luzar, A.
Attractive surface force in the presence of dissolved gas: A molecular approach
(2008) *Langmuir*, 24 (4), pp. 1247-1253. Cited 41 times.
doi: 10.1021/la702328w
View at Publisher
-
- 21 Peralta, R.A., Alcántar-Vázquez, B., Sánchez-Serratos, M., González-Zamora, E., Ibarra, I.A.
Carbon dioxide capture in the presence of water vapour in InOF-1
(2015) *Inorganic Chemistry Frontiers*, 2 (10), pp. 898-903. Cited 23 times.
<http://pubs.rsc.org/en/journals/journal/qi>
doi: 10.1039/c5qi00077g
View at Publisher
-
- 22 Gonzalez, M.R., González-Estefan, J.H., Lara-García, H.A., Sánchez-Camacho, P., Basaldella, E.I., Pfeiffer, H., Ibarra, I.A.
Separation of CO₂ from CH₄ and CO₂ capture in the presence of water vapour in NOTT-400
(2015) *New Journal of Chemistry*, 39 (4), pp. 2400-2403. Cited 24 times.
<http://pubs.rsc.org/en/journals/journal/nj>
doi: 10.1039/c4nj01933d
View at Publisher
-
- 23 Sagastuy-Breña, M., Mileo, P.G.M., Sánchez-González, E., Reynolds, J.E., Jurado-Vázquez, T., Balmaseda, J., González-Zamora, E., (...), Ibarra, I.A.
Humidity-induced CO₂ capture enhancement in Mg-CUK-1
(2018) *Dalton Transactions*, 47 (44), pp. 15827-15834. Cited 4 times.
<http://pubs.rsc.org/en/journals/journal/dt>
doi: 10.1039/c8dt03365j
View at Publisher
-
- 24 González-Zamora, E., Ibarra, I.A.
CO₂ capture under humid conditions in metal-organic frameworks
(2017) *Materials Chemistry Frontiers*, 1 (8), pp. 1471-1484. Cited 42 times.
rsc.li/frontiers-materials
doi: 10.1039/c6qm00301j
View at Publisher

- 25 Zárate, J.A., Sánchez-González, E., Williams, D.R., González-Zamora, E., Martis, V., Martínez, A., Balmaseda, J., (...), Ibarra, I.A.

High and energy-efficient reversible SO₂ uptake by a robust Sc(III)-based MOF

(2019) *Journal of Materials Chemistry A*, 7 (26), pp. 15580-15584. Cited 7 times.

<http://pubs.rsc.org/en/journals/journal/ta>

doi: 10.1039/c9ta02585e

[View at Publisher](#)

- 26 Qian, J., Jiang, F., Yuan, D., Wu, M., Zhang, S., Zhang, L., Hong, M.

Highly selective carbon dioxide adsorption in a water-stable indium-organic framework material

(2012) *Chemical Communications*, 48 (78), pp. 9696-9698. Cited 113 times.

doi: 10.1039/c2cc35068h

[View at Publisher](#)

- 27 Savage, M., Cheng, Y., Easun, T.L., Eyley, J.E., Argent, S.P., Warren, M.R., Lewis, W., (...), Schröder, M.

Selective Adsorption of Sulfur Dioxide in a Robust Metal–Organic Framework Material ([Open Access](#))

(2016) *Advanced Materials*, 28 (39), pp. 8705-8711. Cited 65 times.

<http://www3.interscience.wiley.com/journal/119030556/issue>

doi: 10.1002/adma.201602338

[View at Publisher](#)

- 28 Sánchez-González, E., Mileo, P.G.M., Álvarez, J.R., González-Zamora, E., Maurin, G., Ibarra, I.A.

Confined methanol within InOF-1: CO₂ capture enhancement

(2017) *Dalton Transactions*, 46 (44), pp. 15208-15215. Cited 11 times.

<http://www.rsc.org/Publishing/Journals>

doi: 10.1039/c7dt02709e

[View at Publisher](#)

- 29 González-Zamora, E., Zárate, J.A., Balmaseda, J., Jancik, V., Álvarez, J.R., Ibarra, I.A., Campos-Reales-Pineda, A., (...), Pfeiffer, H.

(2016) *Chem. Commun.*, 52, pp. 10273-10276.

- 30 Raziel Álvarez, J., Mileo, P.G.M., Sánchez-González, E., Antonio Zárate, J., Rodríguez-Hernández, J., González-Zamora, E., Maurin, G., (...), Ibarra, I.A.

Adsorption of 1-Propanol in the Channel-Like InOF-1 Metal–Organic Framework and Its Influence on the CO₂ Capture Performances

(2018) *Journal of Physical Chemistry C*, 122 (10), pp. 5566-5577. Cited 10 times.

<http://pubs.acs.org/journal/jpcck>

doi: 10.1021/acs.jpcc.8b00215

[View at Publisher](#)

- 31 Sánchez-Bautista, J.E., Landeros-Rivera, B., Jurado-Vázquez, T., Martínez, A., González-Zamora, E., Balmaseda, J., Vargas, R., (...), Ibarra, I.A.

CO₂ capture enhancement for InOF-1: confinement of 2-propanol

(2019) *Dalton Transactions*, 48 (16), pp. 5176-5182. Cited 2 times.

<http://pubs.rsc.org/en/journals/journal/dt>

doi: 10.1039/c9dt00384c

[View at Publisher](#)

- 32 Sánchez-González, E., González-Zamora, E., Martínez-Otero, D., Jancik, V., Ibarra, I.A.
Bottleneck Effect of N,N-Dimethylformamide in InOF-1: Increasing CO₂ Capture in Porous Coordination Polymers

(2017) *Inorganic Chemistry*, 56 (10), pp. 5863-5872. Cited 16 times.

<http://pubs.acs.org/journal/inocaj>

doi: 10.1021/acs.inorgchem.7b00519

[View at Publisher](#)

- 33 Garrido-Olvera, L.P., Sanchez-Bautista, J.E., Alvarado-Alvarado, D., Landeros-Rivera, B., Álvarez, J.R., Vargas, R., González-Zamora, E., (...), Ibarra, I.A.

Confined toluene within InOF-1: CO₂ capture enhancement ([Open Access](#))

(2019) *RSC Advances*, 9 (56), pp. 32864-32872.

<http://pubs.rsc.org/en/journals/journal/ra>

doi: 10.1039/c9ra05991a

[View at Publisher](#)

- 34 Civalleri, B., Zicovich-Wilson, C.M., Valenzano, L., Ugliengo, P.
B3LYP augmented with an empirical dispersion term (B3LYP-D*) as applied to molecular crystals

(2008) *CrystEngComm*, 10 (4), pp. 405-410. Cited 467 times.

<http://pubs.rsc.org/en/journals/journal/ce>

doi: 10.1039/b715018k

[View at Publisher](#)

- 35 Peintinger, M.F., Oliveira, D.V., Bredow, T.
Consistent Gaussian basis sets of triple-zeta valence with polarization quality for solid-state calculations

(2013) *Journal of Computational Chemistry*, 34 (6), pp. 451-459. Cited 455 times.

doi: 10.1002/jcc.23153

[View at Publisher](#)

- 36 Dovesi, R., Orlando, R., Erba, A., Zicovich-Wilson, C.M., Civalleri, B., Casassa, S., Maschio, L., (...), Kirtman, B.

C RYDAL14: A program for the ab initio investigation of crystalline solids

(2014) *International Journal of Quantum Chemistry*, 114 (19), pp. 1287-1317. Cited 880 times.

[http://onlinelibrary.wiley.com/journal/10.1002/\(ISSN\)1097-461X](http://onlinelibrary.wiley.com/journal/10.1002/(ISSN)1097-461X)

doi: 10.1002/qua.24658

[View at Publisher](#)

- 37 Bader, R.F.W.
(1990) *Atoms in Molecules: A Quantum Theory*. Cited 15369 times.
Oxford University Press, Oxford

- 38 Hernández-Esparza, R., Mejía-Chica, S.-M., Zapata-Escobar, A.D., Guevara-García, A., Martínez-Melchor, A., Hernández-Pérez, J.-M., Vargas, R., (...), Garza, J.

Grid-based algorithm to search critical points, in the electron density, accelerated by graphics processing units

(2014) *Journal of Computational Chemistry*, 35 (31), pp. 2272-2278. Cited 22 times.

[http://onlinelibrary.wiley.com/journal/10.1002/\(ISSN\)1096-987X](http://onlinelibrary.wiley.com/journal/10.1002/(ISSN)1096-987X)

doi: 10.1002/jcc.23752

[View at Publisher](#)

- 39 Szostak, R.
(1992) *Handbook of Molecular Sieves: Structures*. Cited 431 times.
Springer
-
- 40 Zhao, Z., Wang, S., Yang, Y., Li, X., Li, J., Li, Z.
Competitive adsorption and selectivity of benzene and water vapor on the microporous metal organic frameworks (HKUST-1)
(2015) *Chemical Engineering Journal*, 259, pp. 79-89. Cited 93 times.
www.elsevier.com/locate/cej
doi: 10.1016/j.cej.2014.08.012
View at Publisher
-
- 41 Sánchez-Bautista, J.E., Landeros-Rivera, B., Jurado-Vázquez, T., Martínez, A., González-Zamora, E., Balmaseda, J., Vargas, R., (...), Ibarra, I.A.
CO₂ capture enhancement for InOF-1: confinement of 2-propanol
(2019) *Dalton Transactions*, 48 (16), pp. 5176-5182. Cited 2 times.
<http://pubs.rsc.org/en/journals/journal/dt>
doi: 10.1039/c9dt00384c
View at Publisher
-
- 42 Lara-García, H.A., Landeros-Rivera, B., González-Zamora, E., Aguilar-Pliego, J., Gómez-Cortés, A., Martínez, A., Vargas, R., (...), Ibarra, I.A.
Relevance of hydrogen bonding in CO₂ capture enhancement within InOF-1: An energy and vibrational analysis
(2019) *Dalton Transactions*, 48 (24), pp. 8611-8616. Cited 2 times.
<http://pubs.rsc.org/en/journals/journal/dt>
doi: 10.1039/c9dt01266d
View at Publisher
-
- 43 Chen, L., Cao, F., Sun, H.
Ab initio study of the π - π Interactions between CO₂ and benzene, pyridine, and pyrrole
(2013) *International Journal of Quantum Chemistry*, 113 (20), pp. 2261-2266. Cited 28 times.
doi: 10.1002/qua.24444
View at Publisher
-
- 44 Witte, J., Neaton, J.B., Head-Gordon, M.
Assessing electronic structure approaches for gas-ligand interactions in metal-organic frameworks: The CO₂-benzene complex
(2014) *Journal of Chemical Physics*, 140 (10), art. no. 104707. Cited 15 times.
<http://jcp.aip.org/>
doi: 10.1063/1.4867698
View at Publisher
-
- 45 David, J.G., Hallam, H.E.
Infra-red solvent shifts and molecular interactions-X triatomic molecules, CS₂, COS and SO₂
(1967) *Spectrochimica Acta Part A: Molecular Spectroscopy*, 23 (3), pp. 593-603. Cited 35 times.
View at Publisher

- 46 Labarge, M.S., Oh, J.-J., Hillig II, K.W., Kuczkowski, R.L.
The benzene-SO₂ and pyridine-SO₂ complexes

(1989) *Chemical Physics Letters*, 159 (5-6), pp. 559-562. Cited 20 times.
doi: 10.1016/0009-2614(89)87532-3

[View at Publisher](#)

- 47 Cui, G., Lin, W., Ding, F., Luo, X., He, X., Li, H., Wang, C.
Highly efficient SO₂ capture by phenyl-containing azole-based ionic liquids through multiple-site interactions

(2014) *Green Chemistry*, 16 (3), pp. 1211-1216. Cited 64 times.
doi: 10.1039/c3gc41458b

[View at Publisher](#)

- 48 Espinosa, E., Molins, E., Lecomte, C.
Hydrogen bond strengths revealed by topological analyses of experimentally observed electron densities

(1998) *Chemical Physics Letters*, 285 (3-4), pp. 170-173. Cited 1831 times.
<http://www.elsevier.com.ezproxy.ulima.edu.pe/locate/cplonline>
doi: 10.1016/S0009-2614(98)00036-0

[View at Publisher](#)

🔍 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

© Copyright 2020 Elsevier B.V., All rights reserved.

1 of 1

[^ Top of page](#)

About Scopus

[What is Scopus](#)
[Content coverage](#)
[Scopus blog](#)
[Scopus API](#)
[Privacy matters](#)

Language

[日本語に切り替える](#)
[切换到简体中文](#)
[切换到繁體中文](#)
[Русский язык](#)

Customer Service

[Help](#)
[Contact us](#)

ELSEVIER

[Terms and conditions](#) ↗ [Privacy policy](#) ↗

Copyright © Elsevier B.V. ↗. All rights reserved. Scopus® is a registered trademark of Elsevier B.V.

We use cookies to help provide and enhance our service and tailor content. By continuing, you agree to the use of cookies.

 RELX