Fundamental Investigations of Nanostructured Chemical Sensing Layers

Patricia C. Madden[1] , Angela L. Goodman[1] , Paul R. Ohodnicki[1], Sean Sanguinito[1 ,2], Ki-Joong Kim[1 ,2]

[1]US Department of Energy, National Energy Technology Laboratory, Pittsburgh, PA /Morgantown, WV; [2]AECOM Corporation, Pittsburgh, PA.

Research & Innovation Center

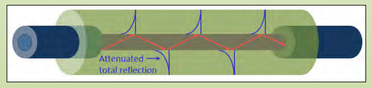
NATIONAL ENERGY TECHNOLOGY LABORATORY

Abstract

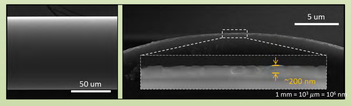
Fiber optic sensors can be coated with metal-organic frameworks (MOFs) to deliver a viable CO_2 sensing technology. This sensing technology is relevant for Carbon Capture and Storage (CCS) where it can be used to monitor CO_2 in geological formations. Fundamental investigations of these nanostructured chemical sensing layers, using Fourier Transform Infrared (FTIR) Spectroscopy, provided validating results of the MOF coated sensor to have a high selectivity to CO_2 relative to other small gases. Research was also conducted to investigate how the presence of a redox-active, conjugated guest molecule affects the MOF's selectivity of CO_2. The MOF under investigation was $Cu_3(BTC)_2$ (benzene-1,2,5-tricarboxylic acid) and the redox-active molecule was TCNQ (7,7,8,8-tetracyanoquinododimetane). This MOF was selected for its high absorption of small gases due to tunable conductivity. The promising results of the project indicate that $Cu_3(BTC)_2$ coated fiber optic sensors can be used not only in optical sensing applications such as monitoring CO_2 in geological formations for CCS, but also in industrial process applications such as monitoring flue gas of power plants.

Project Overview

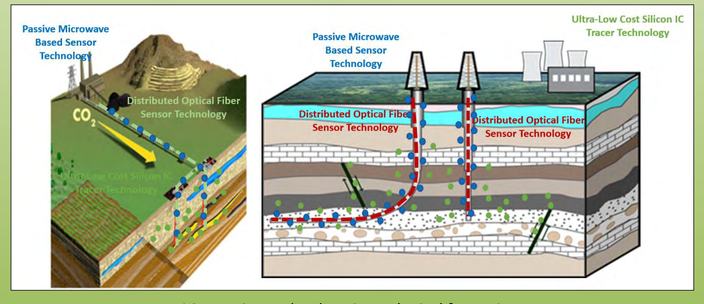
Fiber optic sensors can be coated with metal-organic frameworks (MOFs) to deliver a viable CO_2 sensing technology in geological formations relevant for Carbon Capture and Storage (CCS) applications.



MOF-coated optical fiber



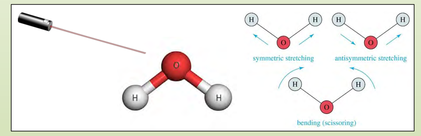
SEM image of MOF-coated optical fiber



CO_2 sensing technology in geological formations

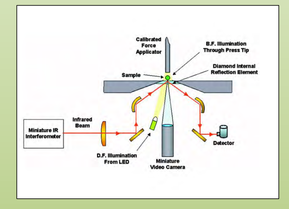
Infrared Spectroscopy

- Infrared spectroscopy analyzes the interaction of infrared light with a molecule.
- The analysis is based on measuring the vibrations of atoms that are specific for each functional group.

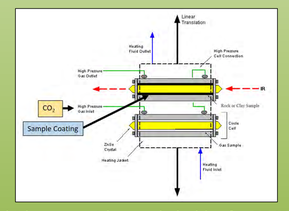


Molecular vibrations detected with IR spectroscopy

FT-IR Spectrometer used to conduct in-situ high temperature and pressure experiments.



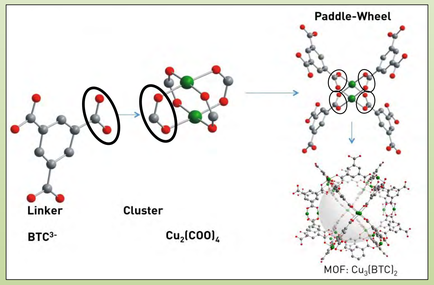
Single bounce ATR

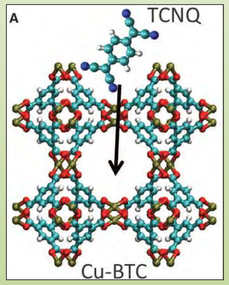


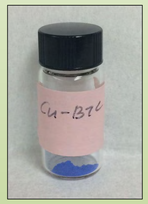
Multi-bounce with sample holder for FT-IR

Metal Organic Framework Synthesis

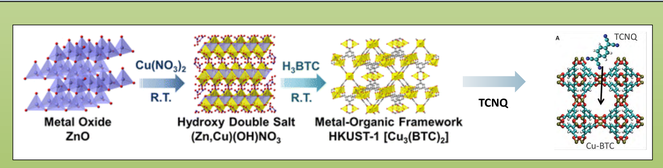
Solvothermal Synthesis Method







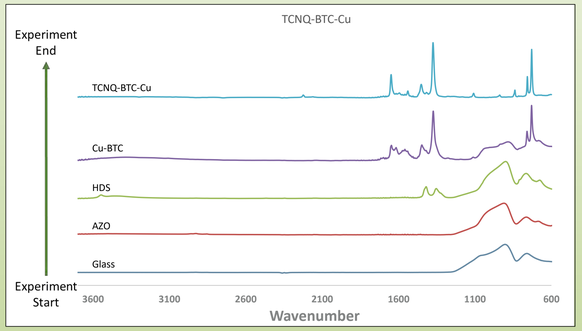
Thin Film Synthesis on Silica Glass Substrate



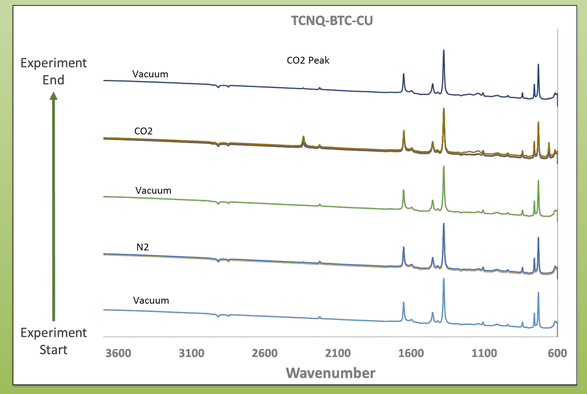
Layer	Thickness (nm)
AZO	120-140
HDS	150-200
Cu-BTC	500-800

Infrared Spectroscopy: Results

Single Bounce ATR



In-situ Multi-Bounce



Conclusions

- IR spectroscopy is part of the tool set
- Provided insight into the selectivity to CO_2 relative to other small gases
- Determined successful synthesis of thin film $Cu_3(BTC)_2$
- MOF coated fiber optic sensors can be used in:
  - Geological formations for CCS
  - Flue gas of power plants
  - Natural gas pipelines

References

- Kim, K.J., Ping, L., Culp, J.T., Ohodnicki, P.R., 2018. Metal-organic framework thin film coated optical fiber sensors: a novel waveguide-based chemical sensing platform. ACS Sensors, v. 3, p. 386-394.
- Talin, A.A., Centrone, A., Ford, A.C., Foster, M.E., Stavila, V., Haney, P., Kinney, R.A., Szalai, V., Gabaly, F.E., Yoon, H.P., Leonard, F., Allendorf, M.D., 2014. Tunable electrical conductivity in metal-organic framework thin-film devices. Science, v. 343, p. 66-69.
- Goodman, A. Nanomaterial Enabled Chemical Sensors for Environmental Monitoring in CO2 Sequestration. Presentation PowerPoint.
- https://www.americanlaboratory.com/914-Application-Notes/19176-Miniaturized-FTIR-for-Maximized-Productivity/
- http://www.int.laborundmore.com/archive/620180/Metal-organic-frameworks%3A-record-breakers-in-porosity.html
- http://www.x-mol.com/paper/53511
- https://en.wikipedia.org/wiki/Infrared_spectroscopy

Acknowledgements

- U.S. Department of Energy, National Energy Technology Laboratory
- Oak Ridge Associated Universities
- Oak Ridge Institute for Science and Education
- Samples prepared by Ki-Joong Kim
- Poster prepared August 8 ,2018

U.S. DEPARTMENT OF ENERGY

This project was funded by the Department of Energy, National Energy Technology Laboratory, an agency of the United States Government, through a support contract with AECOM. Neither the United States Government nor any agency thereof, nor any of their employees, nor AECOM, nor any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Science & Engineering To Power Our Future