## 4A Water Treatment I

| | | |
| --- | --- | --- |
| 10:30 AM | Multifunctional magnetic nanocomposites (Overview talk) | Dino Villagran |
| 11:00 AM | Arsenic Removal by Graphene Oxide-Nanoscale Zero-valent Iron Hybrid | Tonoy K. Das |
| 11:20 AM | Development of multifunctional nanocomposite coating for indirect potable reuse water treatment | Pasan Chinthana Bandara |
| 11:40 AM | Producing Clean Water and Salinity Gradient Energy by Using a Graphene Oxide Laminate | Xin Tong |
| 12:00 PM | Iron Nanoparticle Impregnated 1-D and 2-D Carbon Nanohybrids Prepared with Ultrasonic Spray Pyrolysis for Cr (VI) Removal | Nirupam Aich |
| 12:20 PM | Investigating the effect of graphene oxide on scaling in thin-film composite polyamide reverse osmosis membranes | Ali Ansari |
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## 4B Water Treatment II

| | | |
| --- | --- | --- |
| 2:00 PM | Preferential interaction between functionalized multiwalled carbon nanotubes and bacteriophage MS2 in water | Navid B. Saleh |
| 2:30 PM | Integration of graphene oxide in mixed-matrix membranes: balancing membrane performance with fouling resistance | Francois Perreault |
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| 3:10 PM | Water Clusters with Superatom Electronic States | Juan C. Noveron |
| 3:40 PM | Break | |
| 4:00 PM | Role of Particle Chemistry on Filtration Mechanisms of Water Treatment- Food Grade and Industrial Grade TiO2 | Chen Chen |
| 4:20 PM | Antimicrobial Property of MoS2 Nanosheets and Potential Application in Controlling Membrane Biofouling | Yingcan Zhao |
| 4:40 PM | Characterizing Wastewater Behavior of Titanium Dioxide Nanoparticles | Travis Waller |
| 5:10 PM | Facile Modification of Bi2WO6 with Base for Improved Photocatalytic Activity under Visible Light | Bangxing Ren |
| 5:30 PM | Quantitative Understanding of Nanoparticle Flocculation in Water Treatment | Sungmin Youn |

# Water Treatment, Overview

- Clean water, one of the most basic needs
- Each year, the world generates 400 billion tons of industrial waste.
- 1.1 billion people do not have access to clean water.
- Social, Agricultural and Environmental issues.

The Global Challenge: Access to Clean, Fresh Water - Institute for Molecular Engineering http://ime.uchicago.edu/features/the_global_challenge_access_to_clean_fresh_water/ (accessed Dec 13, 2016).
2013 - United Nations International Year of Water Cooperation: Facts and Figures http://www.unwater.org/water-cooperation-2013/water-cooperation/facts-and-figures/en/ (accessed Dec 13, 2016).

# Global... and local


# Nanotechnology can enhance existing treatment processes

- Turbidity, Taste/odor — Selective adsorbents
- Water hardness — Electrosorption
- Heavy metal contaminants — Selective adsorbents, Catalysis, Membranes
- Oxoanions — Selective adsorbents, Catalysis
- Organic pollutants (pesticides, endocrine disruptors, pharmaceuticals) — Selective adsorbents, Catalysis, Photocatalysis
- Salts — Electrosorption, Membranes, Distillation
- Pathogens — Catalysis, Photocatalysis

# Multifunctional Magnetic Porous Nanocomposites For Water Treatment

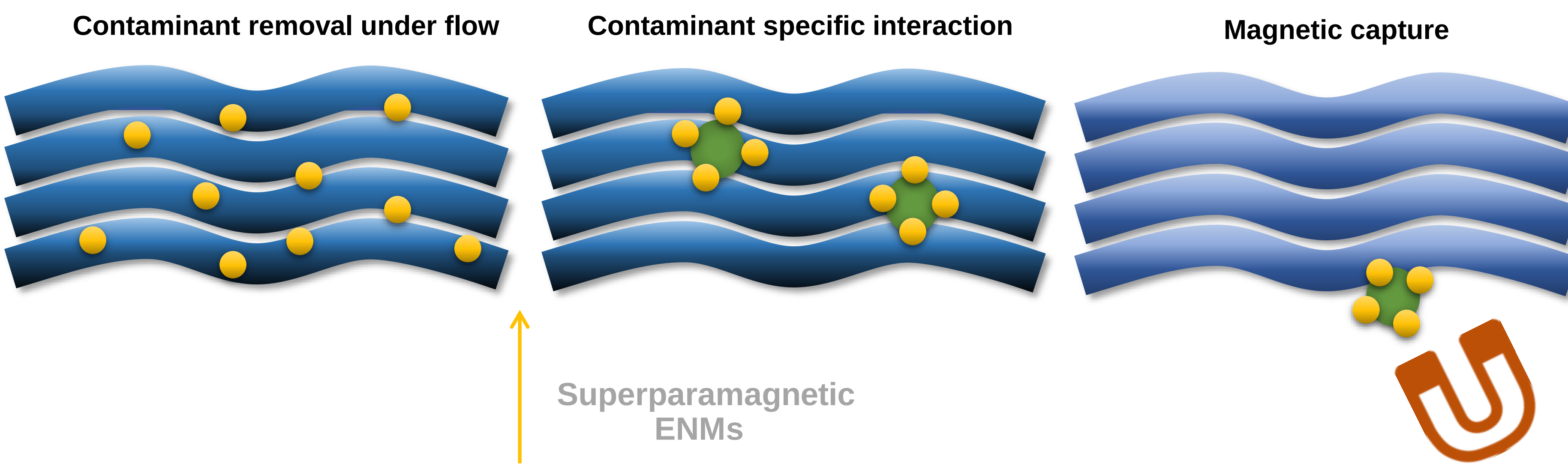
Dino Villagran

Students: Karen Ventura, Roy Arrieta, Vahid Jabbari, Mariana Marcos

The University of Texas at El Paso
Chemistry Department

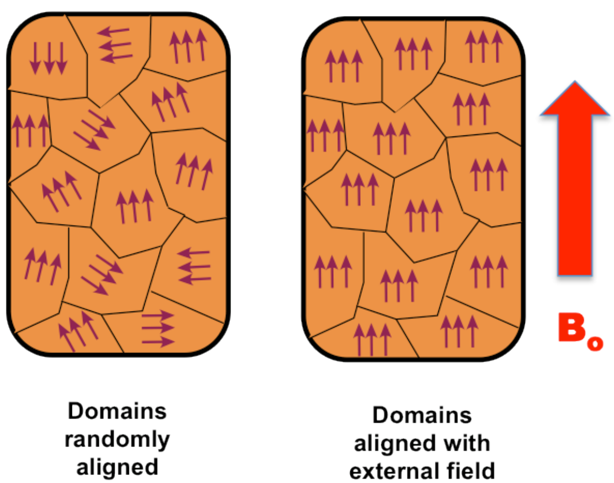
November 6th, 2017

# Magnetic nanomaterials




Contaminant binds to $Fe_3O_4$ nanoparticles

Low-field magnet traps nanoparticles

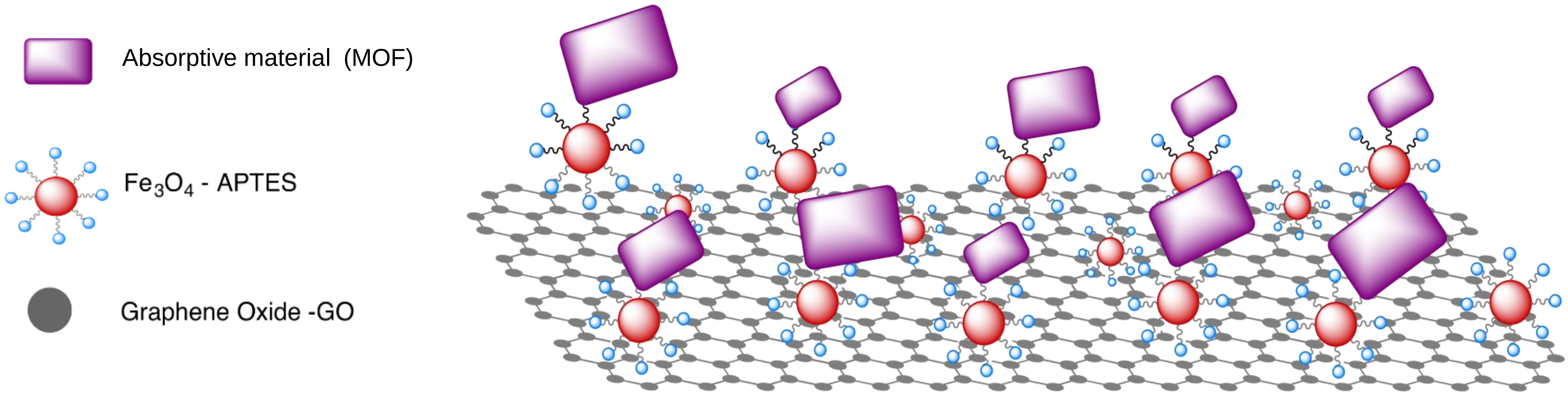


# Objective

Synthesize engineered nanomaterials with enhanced absorptive properties

Build a composite system that has these properties

- High Stability
- High Absorptivity towards water pollutants
- Magnetic



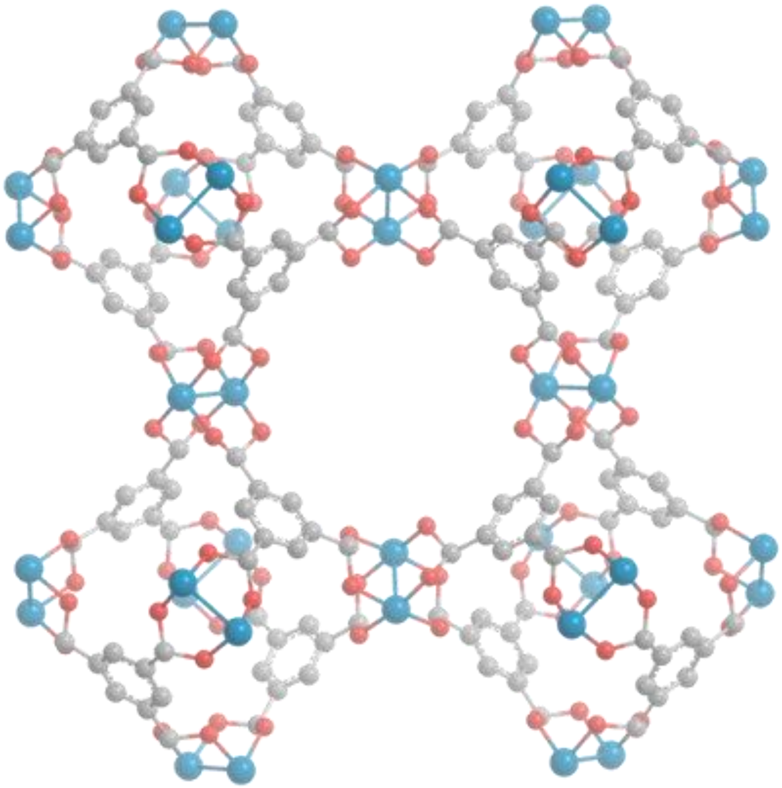
# Metal Organic Frameworks (or ZIFs)

2 gram
MOF-5

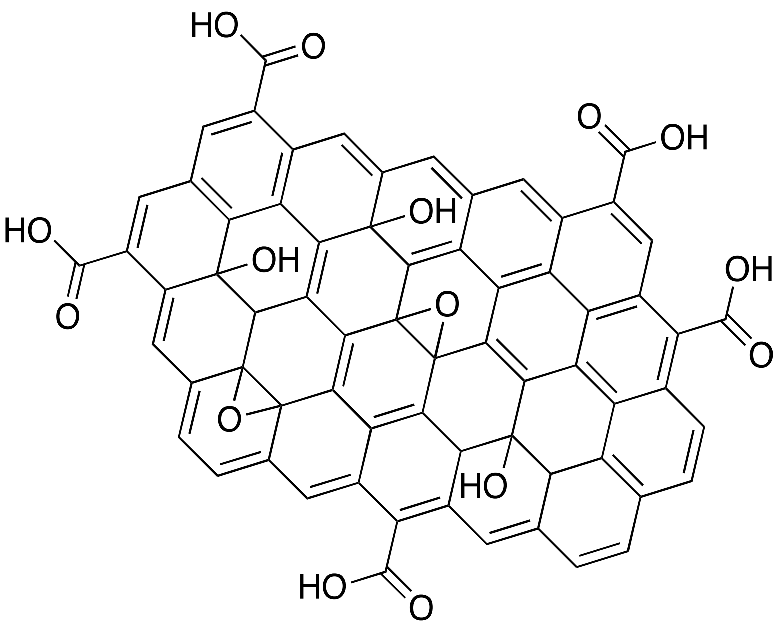
2,900 $m^2/g$
Surface Area

# Metal-Organic Frameworks and Zeolitic-Imidizolate Frameworks

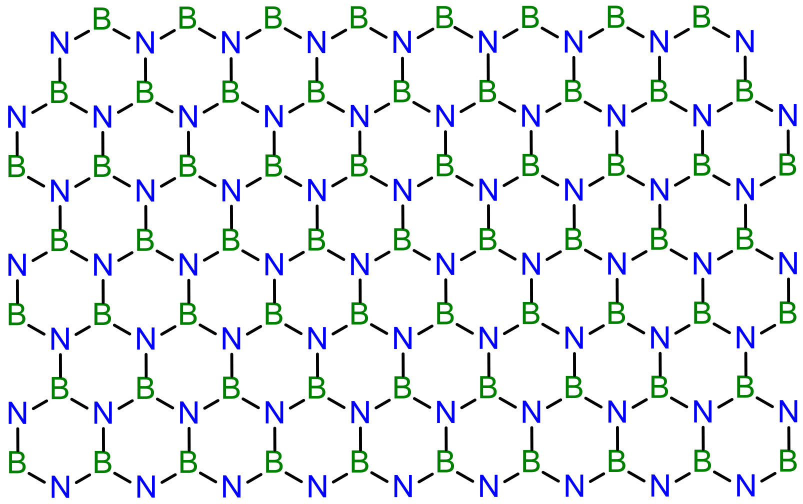
- High porosity
- Thermal stability
- Chemical Stability
- Small molecule absorption
- M = Ni, Cu, Co, Zn, Zr
- HKUST; UiO66;



# Supporting Platforms

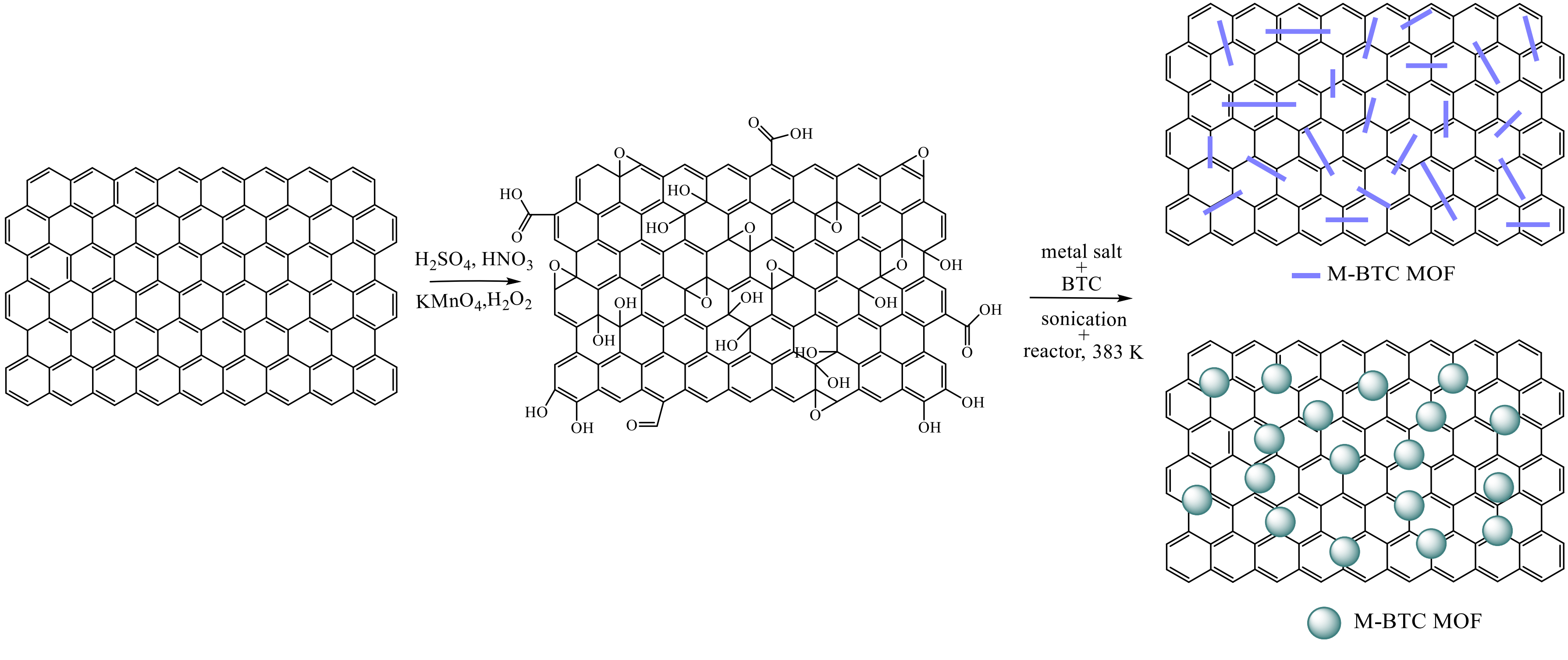


Graphene oxide
(GO)

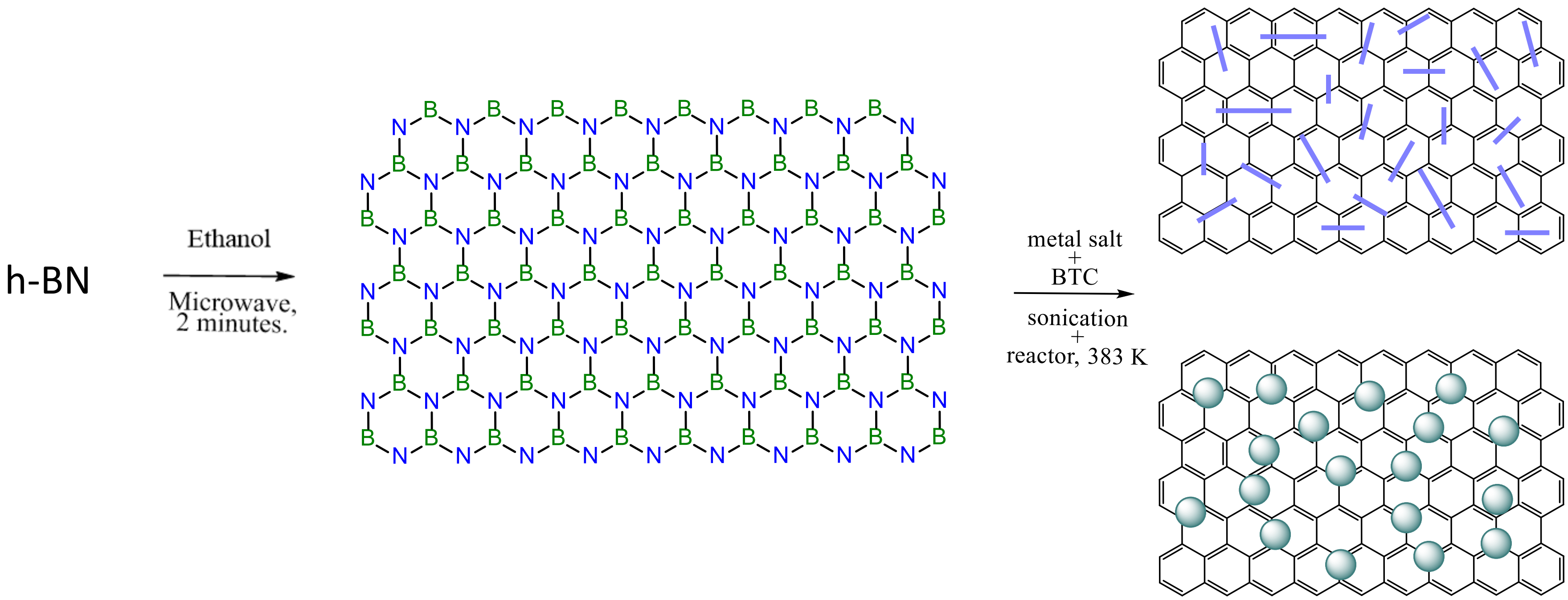


Boron Nitride Nanosheets
(BNNs)

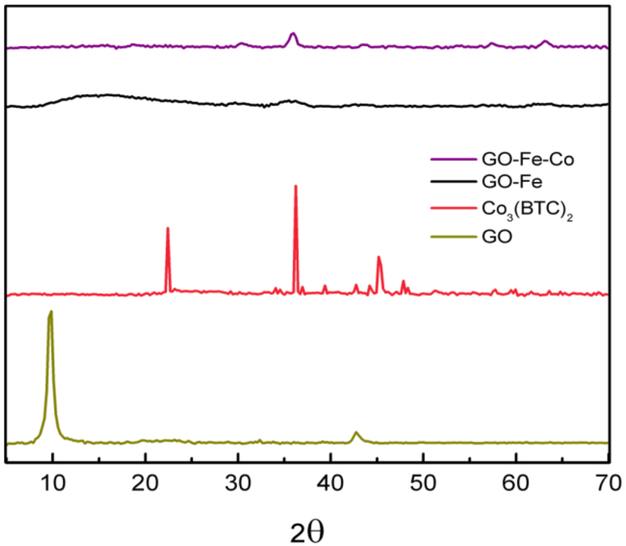
# *in-situ* Formation and Decoration of the MOFs over Graphene Layer

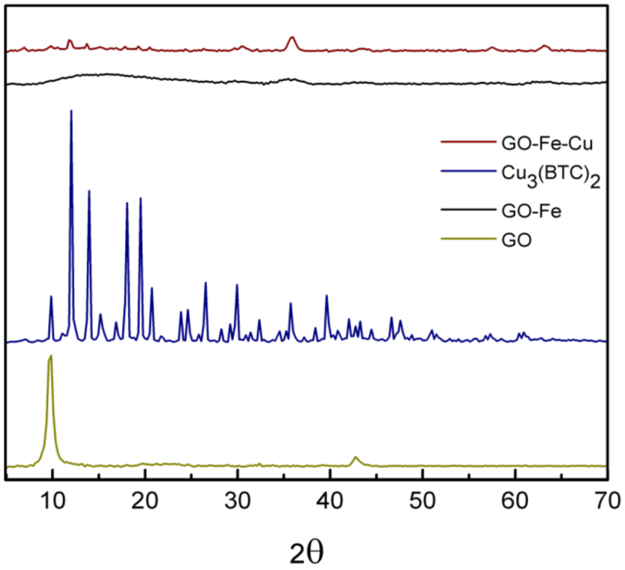


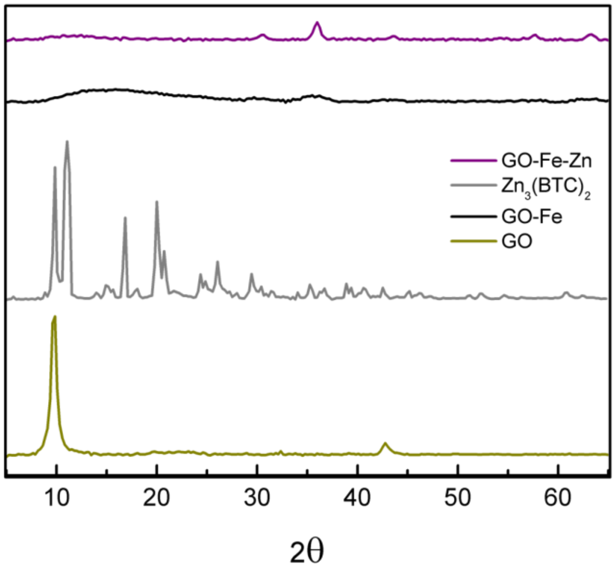

*Chem. Eng. J.*, **2016**, 774-783

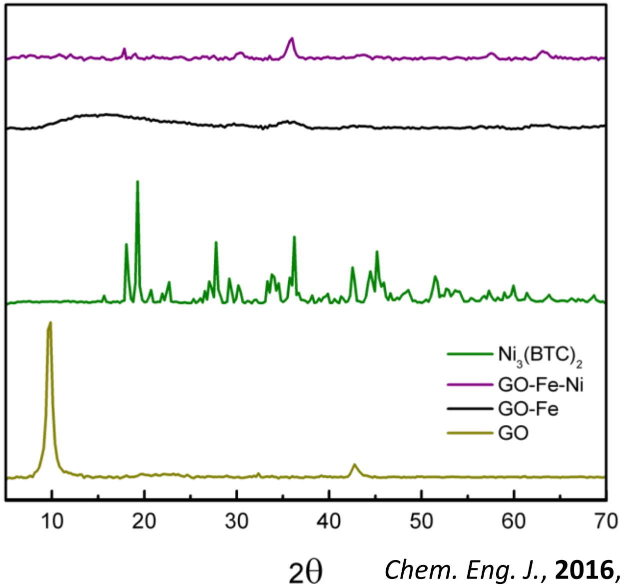

h-BN
Ethanol
Microwave,
2 minutes.
metal salt
+
BTC
sonication
+
reactor, 383 K

# Powder X-Ray Diffraction



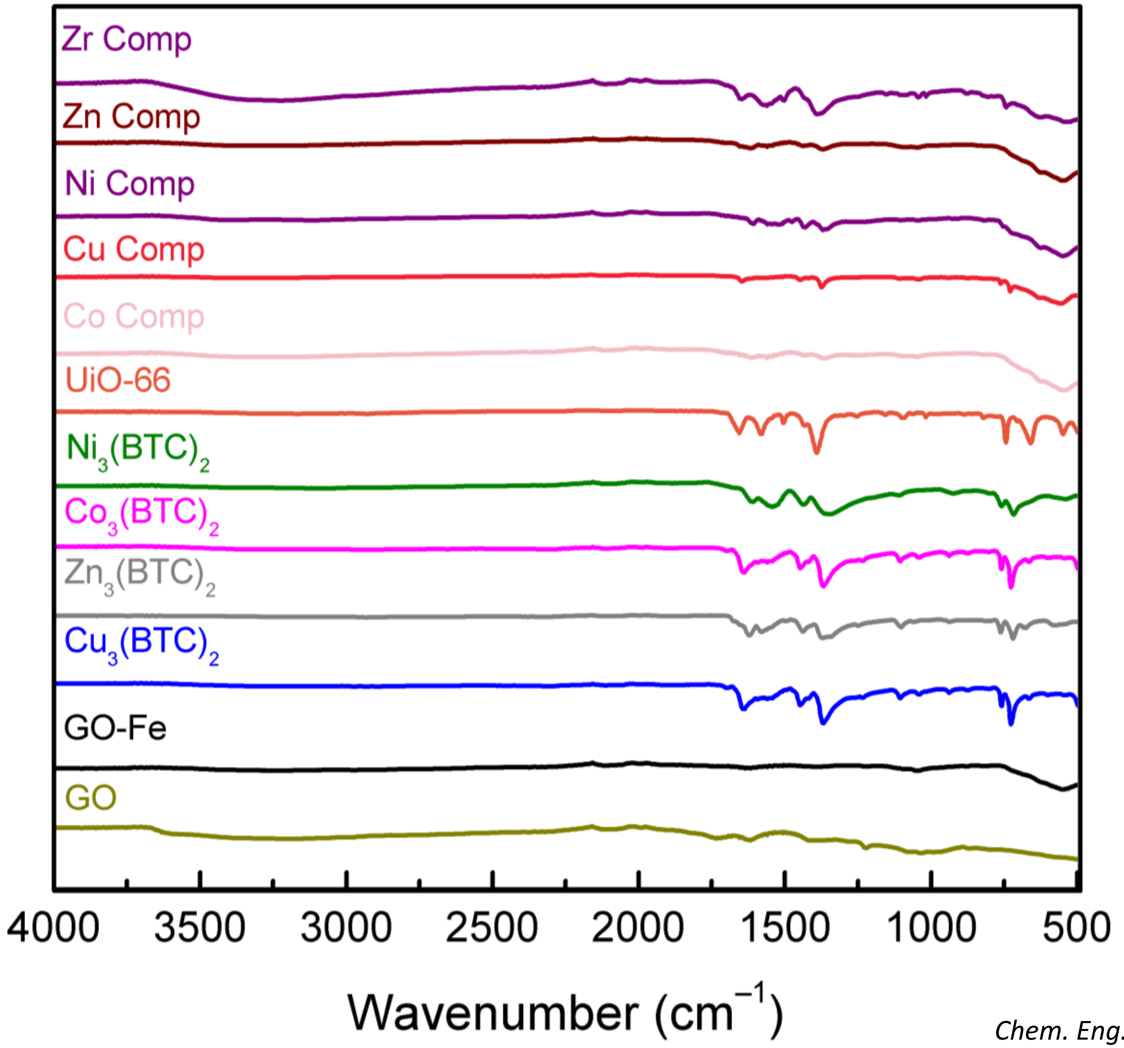





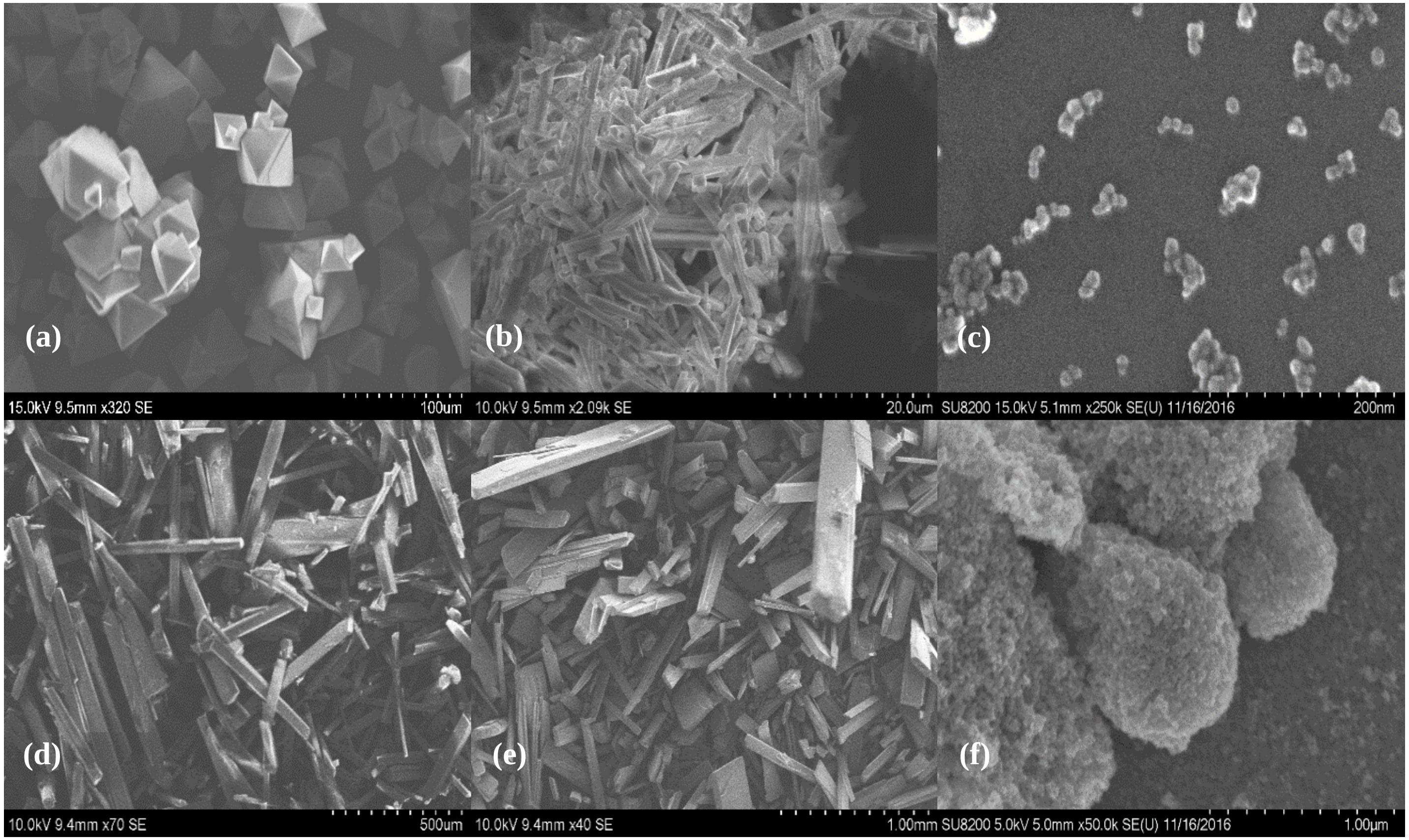

*Chem. Eng. J.*, **2016**, 774-783

# Infra-Red Spectra



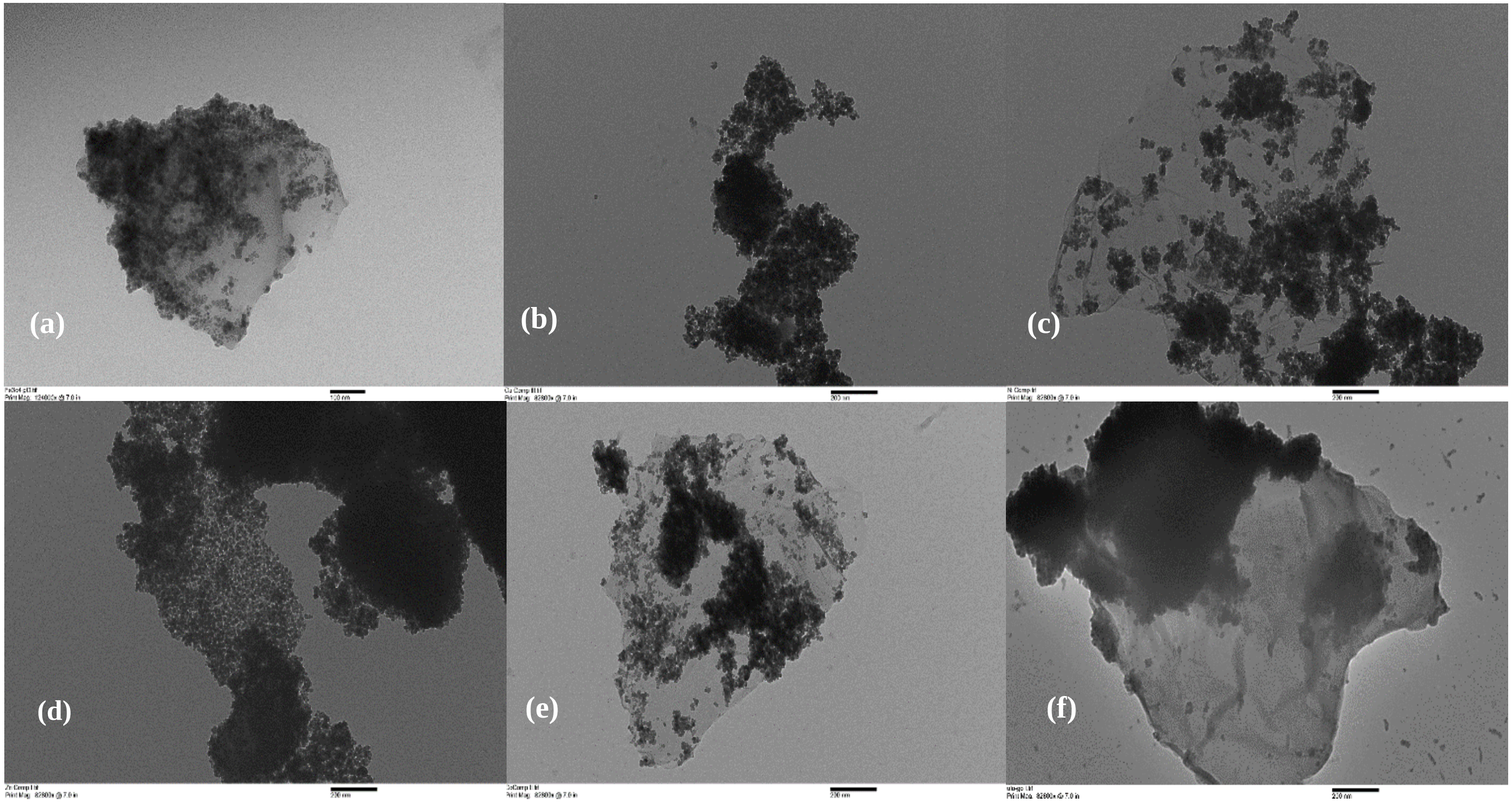

*Chem. Eng. J.*, **2016**, 774-783

# Scanning Electron Microscope



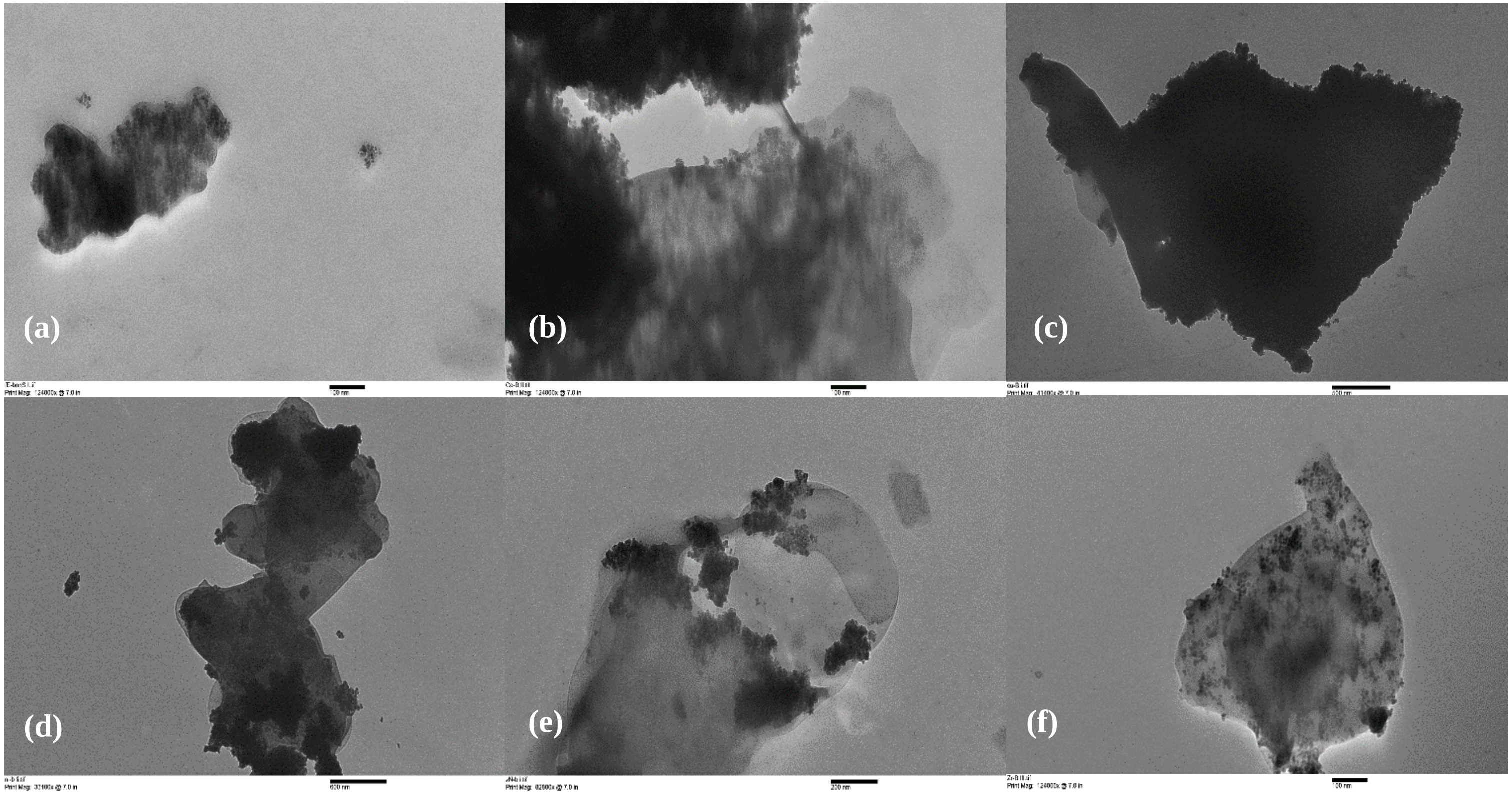

SEM images for parent materials. (a) $Cu_3(BTC)_2$. (b)$Ni_3(BTC)_2$. (c) $Fe_3O_4$ Nanoparticles. (d) $Zn_3(BTC)_2$. (e) $Co_3(BTC)_2$. (f) $Fe_3O_4$ nanoparticles functionalized with APTES.

# Transmission Electron Microscopy




TEM images for GO-nanocomposites. (a) GO coated with $Fe_3O_4$ nanoparticles. (b) GO-$Co_3(BTC)_2$ magnetic nanocompsite. (c) GO-$Cu_3(BTC)_2$ magnetic nanocomposite. (d) GO-$Ni_3(BTC)_2$ magnetic nanocomposite. (e)GO-$Zn_3(BTC)_2$ magnetic nanocomposite. (f) GO-UiO-66 magnetic nanocomposite.

# Transmission Electron Microscope




TEM images for BNNs nanocomposites. (a)BNNs coated with $Fe_3O_4$ nanoparticles. (b)BN-$Co_3(BTC)_2$ magnetic nanocomposite. (c)BN-$Cu_3(BTC)_2$ magnetic nanocomposite. (d) BN-$Ni_3(BTC)_2$ magnetic nancomposite. (e) BN-$Zn_3(BTC)_2$ magnetic nanocomposite. (f) BN-UiO-66 magnetic nanocomposite.

# Scanning Electron Microscope

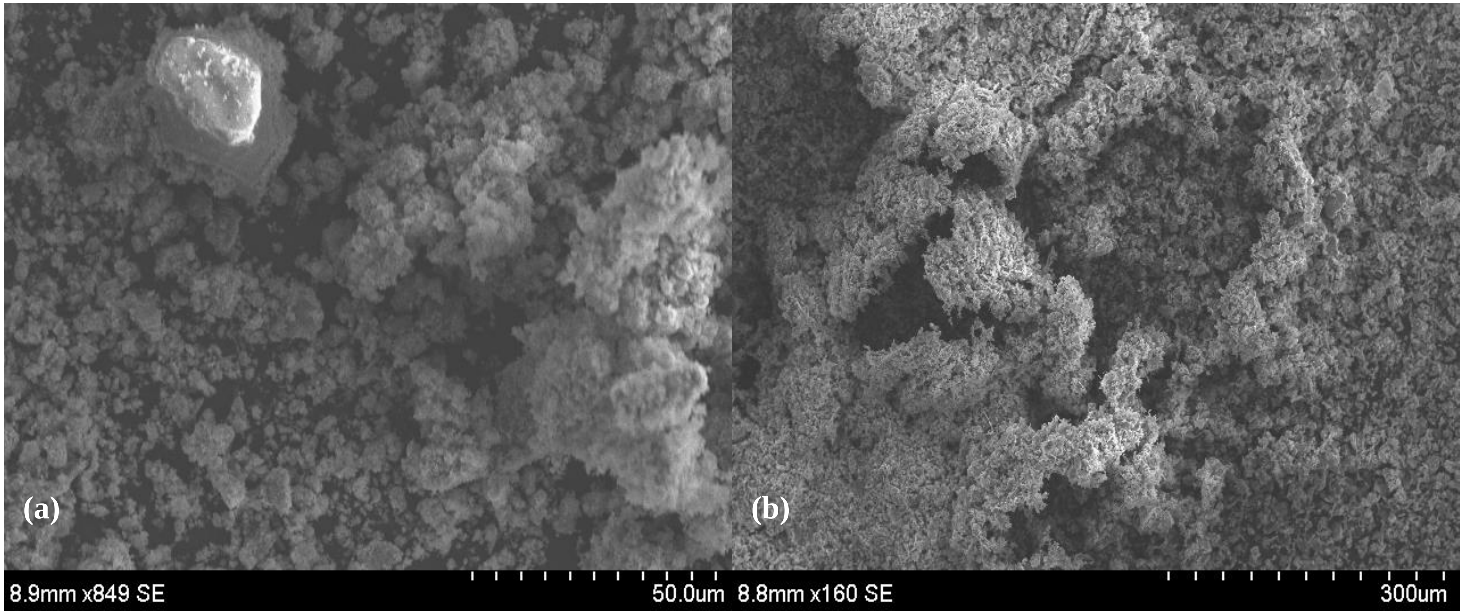
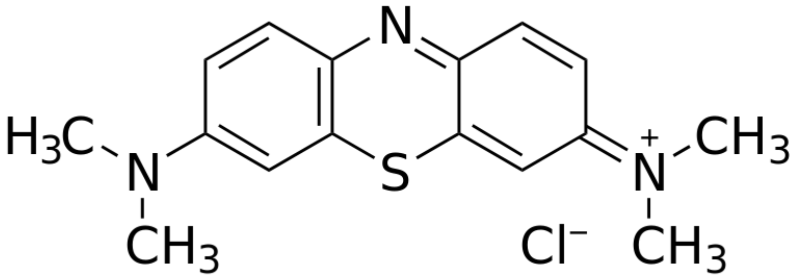



**Figure 15**. SEM of nanocomposites. (a)GO-$Co_3(BTC)_2$ magnetic nanocomposites. (b) BN-$Co_3(BTC)_2$ magnetic nanocomposite.

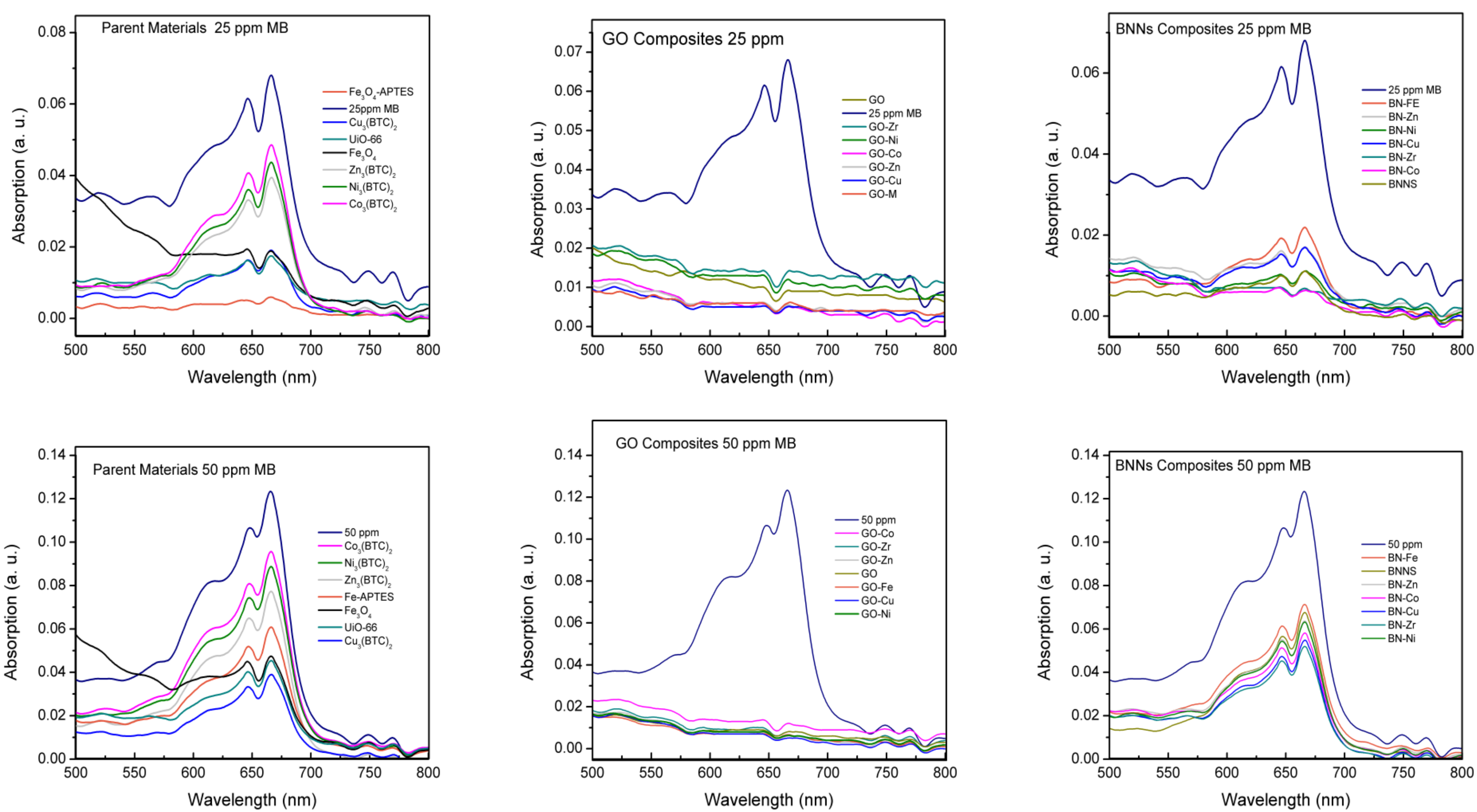
# Methylene Blue (MB)

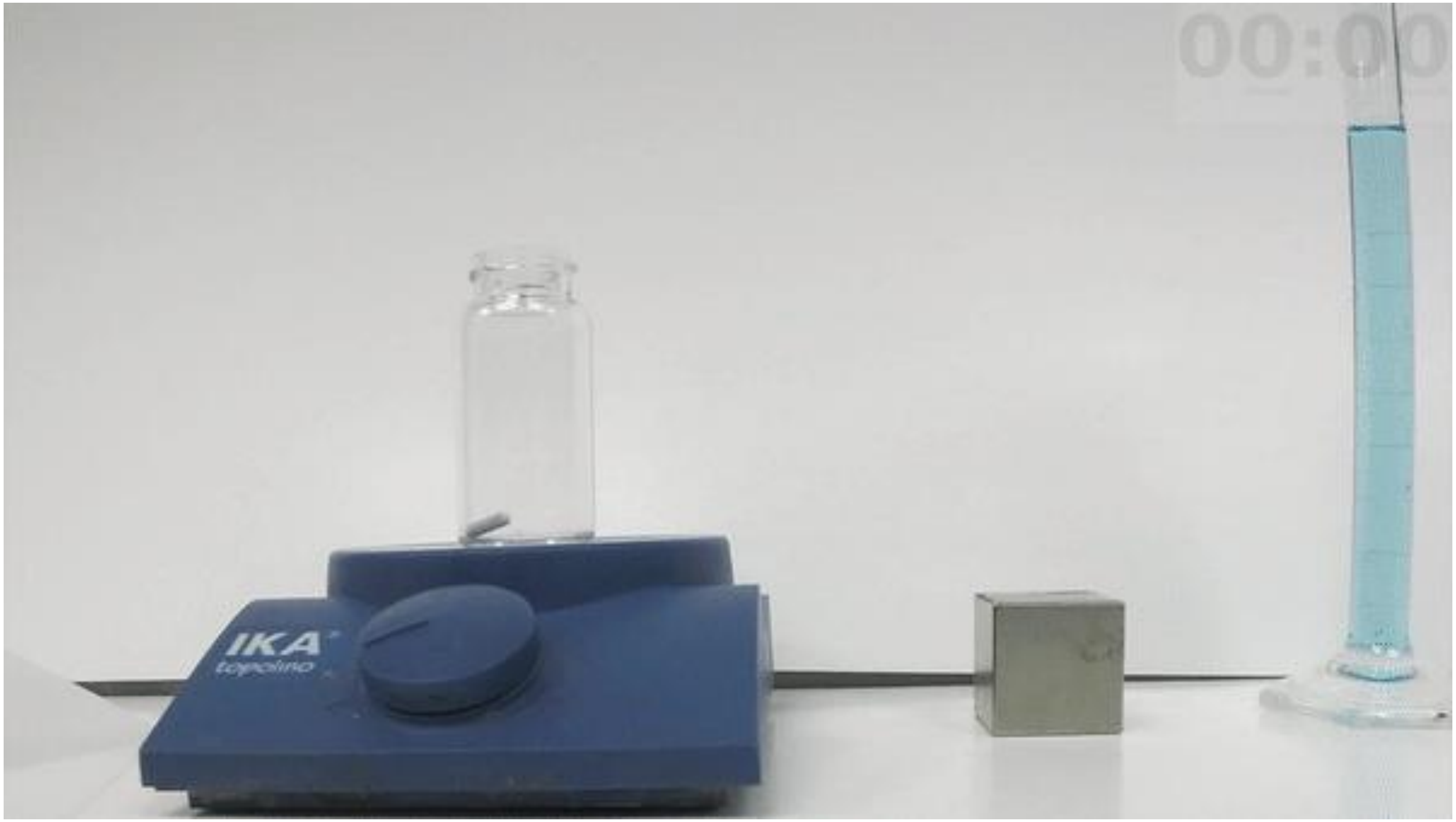
- One of the most common dying materials for textile, MB, has severe health issues such as:
- Neurotoxicity
- Dizziness
- Mental confusion
- Abdominal pain
- Anemia
- Bladder irritation
- Precordial pain



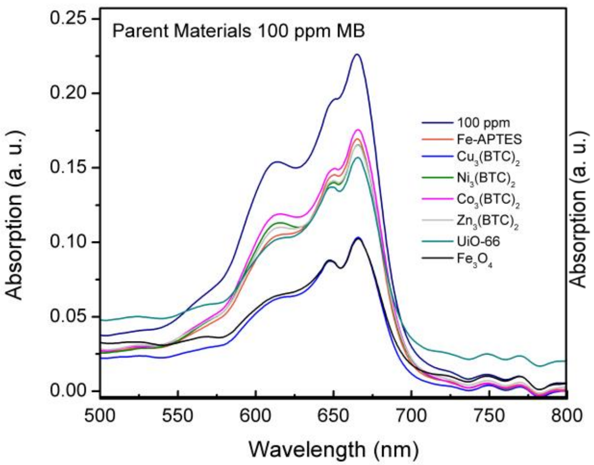

Chemical structure of MB

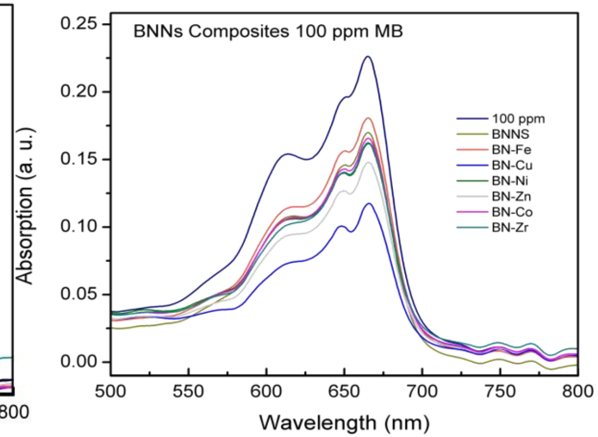
# UV-vis

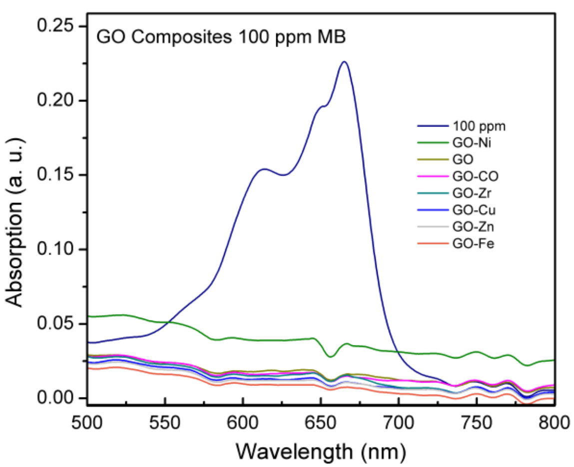

Parent Materials 25 ppm MB
Fe3O4-APTES
25ppm MB
Cu3(BTC)2
UiO-66
Fe3O4
Zn3(BTC)2
Ni3(BTC)2
Co3(BTC)2
Absorption (a. u.)
Wavelength (nm)
GO Composites 25 ppm
GO
25 ppm MB
GO-Zr
GO-Ni
GO-Co
GO-Zn
GO-Cu
GO-M
BNNs Composites 25 ppm MB
25 ppm MB
BN-FE
BN-Zn
BN-Ni
BN-Cu
BN-Zr
BN-Co
BNNS
Parent Materials 50 ppm MB
50 ppm
Co3(BTC)2
Ni3(BTC)2
Zn3(BTC)2
Fe-APTES
Fe3O4
UiO-66
Cu3(BTC)2
GO Composites 50 ppm MB
50 ppm
GO-Co
GO-Zr
GO-Zn
GO
GO-Fe
GO-Cu
GO-Ni
BNNs Composites 50 ppm MB
50 ppm
BN-Fe
BNNS
BN-Zn
BN-Co
BN-Cu
BN-Zr
BN-Ni


00:00
IKA
topolino

# UV-vis

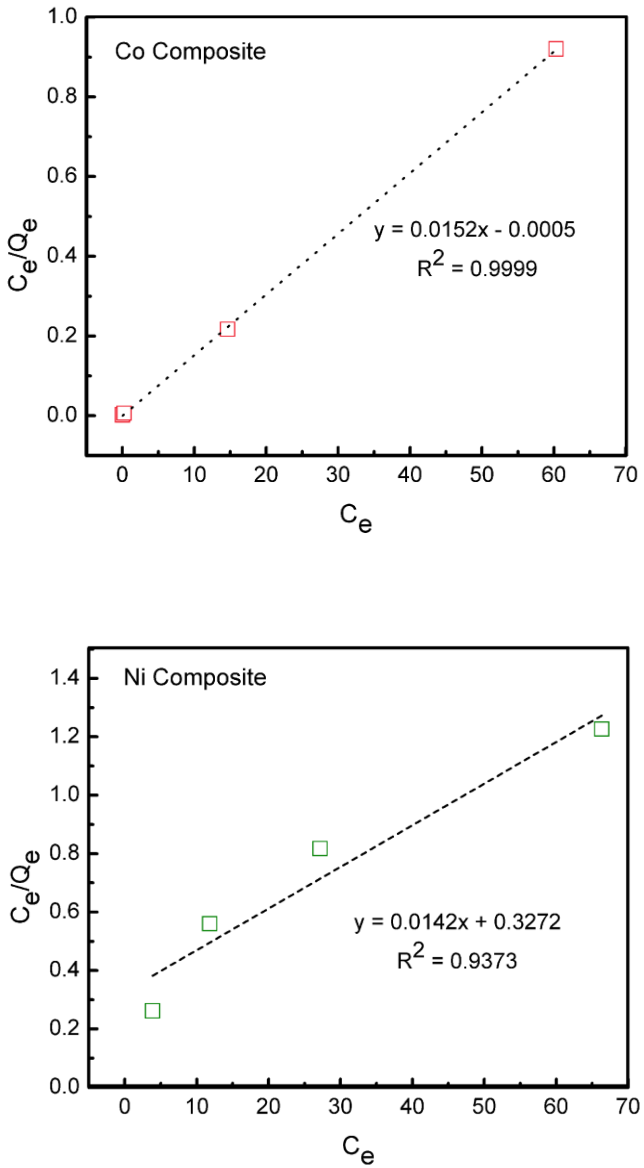


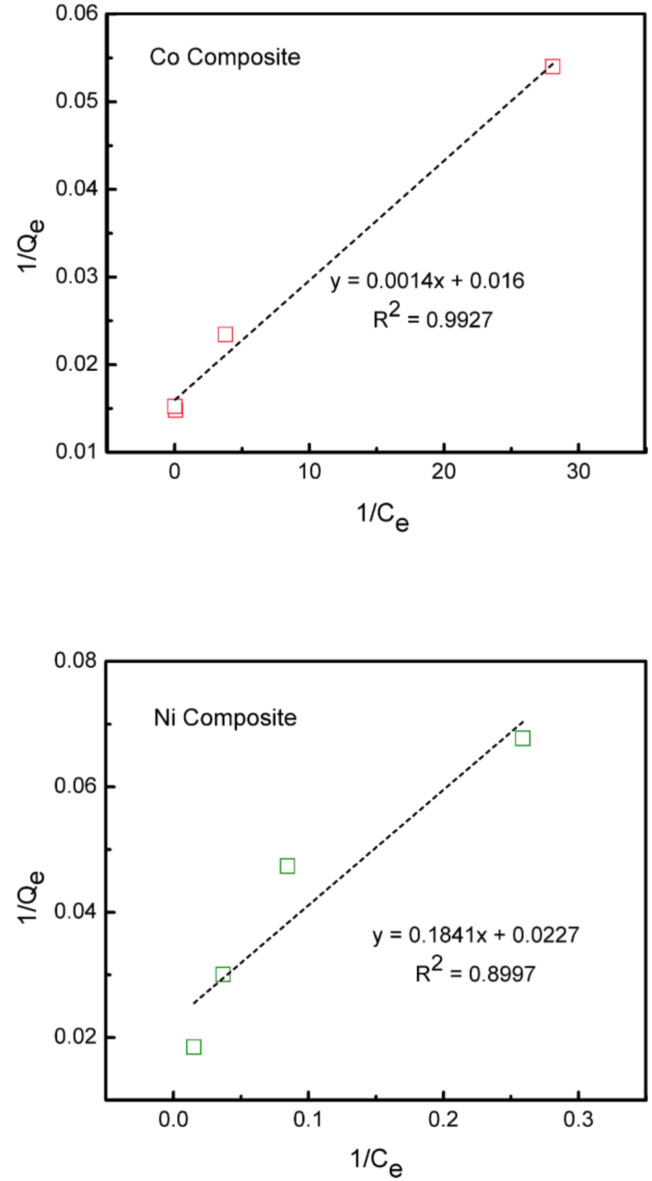




| Salt | Amount mg/L |
|---|---|
| $NaHCO_3$ | 252 |
| $CaCl_2$• 2 $H_2O$ | 147 |
| $MgSO_4$• 7 $H_2O$ | 124 |
| $Na_2SiO_3$• 9 $H_2O$ | 95 |
| $NaNO_3$ | 12 |
| NaF | 2.2 |
| $NaH_2PO_4$• H2O | 0.18 |

| Sample | Qe (mg/g) | | |
|---|---|---|---|
| | 25 ppm | 50 ppm | 100 ppm |
| Fe3O4 | 33.74 | 70.55 | 82.17 |
| Fe-APTES | 39.13 | 51.99 | 52.01 |
| GO | 44.25 | 92.31 | 178.34 |
| BNNs | 43.39 | 38.44 | 55.37 |
| GO-Fe | 48.71 | 89.69 | 153.13 |
| BN-Fe | 35.24 | 40.41 | 50.63 |
| Cu(BTC) | 37.18 | 67.69 | 108.19 |
| Ni(BTC) | 12.25 | 24.58 | 51.41 |
| Co(BTC) | 9.05 | 23.75 | 36.17 |
| Zn(BTC) | 15.36 | 34.62 | 63.71 |
| UiO-66 | 36.57 | 51.47 | 59.32 |
| GO-Cu | 48.61 | 85.01 | 146.51 |
| GO-Ni | 32.71 | 105.29 | 189.76 |
| GO-Zn | 46.80 | 103.98 | 172.67 |
| GO-Co | 54.01 | 92.52 | 146.09 |
| GO-Zr | 37.08 | 84.21 | 157.54 |
| BN-Cu | 38.95 | 54.05 | 89.60 |
| BN-Ni | 33.90 | 53.53 | 57.49 |
| BN-Zn | 30.79 | 51.42 | 77.36 |
| BN-Co | 46.87 | 61.07 | 63.71 |
| BN-Zr | 41.85 | 58.92 | 58.86 |

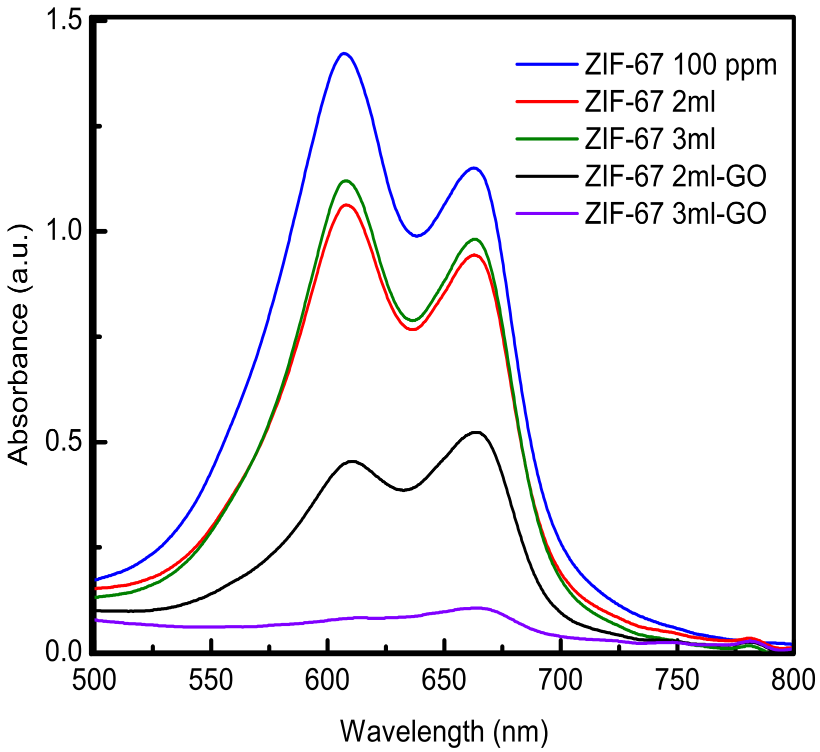



Type I




Type II

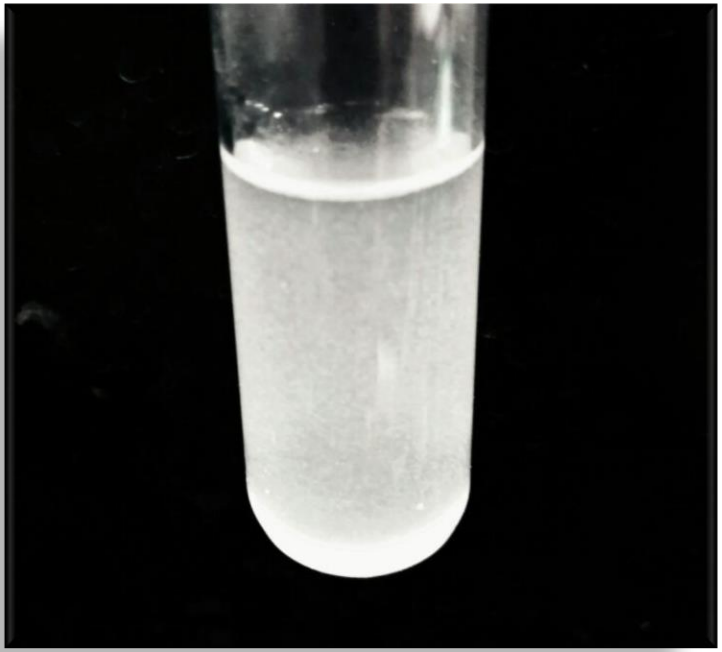
# Zeolitic Imidazolate Frameworks



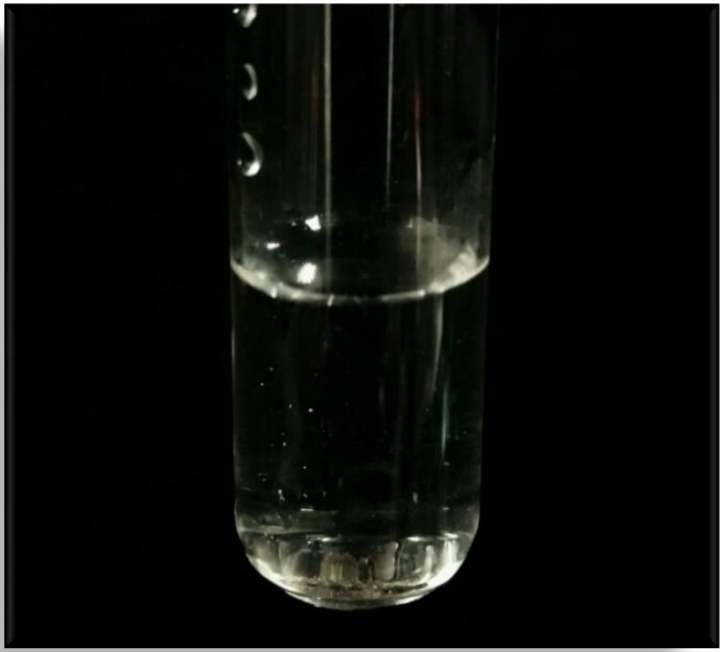

| | 12.5 ppm MB | 25 ppm MB | 50 ppm MB | 100 ppm MB |
|---|---|---|---|---|
| Composite | Avg. Qe. | Avg. Qe. | Avg. Qe. | Avg. Qe |
| ZIF-67 2mL TEA | 15.01 | 18.48 | 30.40 | 28.92 |
| ZIF-67 3mL TEA | 15.91 | 16.48 | 35.80 | 21.89 |
| ZIF-67 2mL TEA/GO | 22.04 | 43.31 | 79.03 | 99.07 |
| ZIF-67 3mL TEA/GO | 22.67 | 37.53 | 78.36 | 120.15 |

# Brackish Water

Before Water Treatment



After Water Treatment



# Brackish Water Treatment

| | | Initial Conc. | average loading (mg/g) | |
|---|---|---|---|---|
| GO | Ca | 158.6 | 58.1 | 94.9 |
| | Ca radial | 158.6 | | |
| | Mg | 52.6 | | |
| | Mg radial | 52.6 | 15.7 | |
| | S | 69.4 | 17.8 | |
| | Si | 9.3 | 3.3 | |
| Fe3O4 | Ca | 158.6 | 53.8 | 124.0 |
| | Ca radial | 158.6 | | |
| | Mg | 52.6 | | |
| | Mg radial | 52.6 | 10.5 | |
| | S | 69.4 | 43.2 | |
| | Si | 9.3 | 16.5 | |
| GO-Fe | Ca | 158.6 | 59.8 | 141.7 |
| | Ca radial | 158.6 | | |
| | Mg | 52.6 | | |
| | Mg radial | 52.6 | 15.6 | |
| | S | 69.4 | 57.7 | |
| | Si | 9.3 | 8.7 | |
| Cu MOF | Ca | 158.6 | 42.3 | 150.4 |
| | Ca radial | 158.6 | | |
| | Mg | 52.6 | | |
| | Mg radial | 52.6 | 14.5 | |
| | S | 69.4 | 83.3 | |
| | Si | 9.3 | 10.4 | |

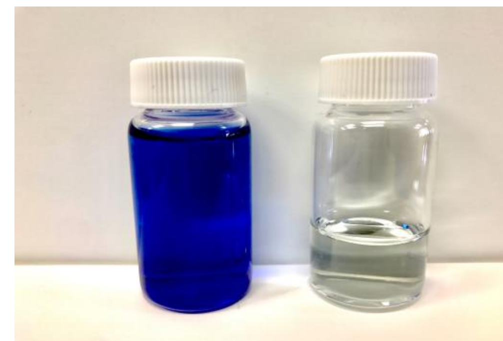
| | | Initial Conc. | average loading (mg/g) | |
|---|---|---|---|---|
| Ni MOF | Ca | 158.6 | 36.0 | 113.0 |
| | Ca radial | 158.6 | | |
| | Mg | 52.6 | | |
| | Mg radial | 52.6 | 9.8 | |
| | S | 69.4 | 59.9 | |
| | Si | 9.3 | 7.3 | |
| Co MOF | Ca | 158.6 | 42.9 | 143.9 |
| | Ca radial | 158.6 | | |
| | Mg | 52.6 | | |
| | Mg radial | 52.6 | 10.6 | |
| | S | 69.4 | 79.4 | |
| | Si | 9.3 | 11.0 | |
| Zn MOF | Ca | 158.6 | 35.0 | 149.2 |
| | Ca radial | 158.6 | | |
| | Mg | 52.6 | | |
| | Mg radial | 52.6 | 11.4 | |
| | S | 69.4 | 93.7 | |
| | Si | 9.3 | 9.1 | |
| UiO-66 | Ca | 158.6 | 55.4 | 206.9 |
| | Ca radial | 158.6 | | |
| | Mg | 52.6 | | |
| | Mg radial | 52.6 | 13.8 | |
| | S | 69.4 | 110.5 | |
| | Si | 9.3 | 27.3 | |

| | | Initial Conc. | average loading (mg/g) | |
|---|---|---|---|---|
| Cu Comp | Ca | 158.6 | 40.2 | 179.7 |
| | Ca radial | 158.6 | | |
| | Mg | 52.6 | | |
| | Mg radial | 52.6 | 13.4 | |
| | S | 69.4 | 112.2 | |
| | Si | 9.3 | 13.9 | |
| Ni Comp | Ca | 158.6 | 64.1 | 223.7 |
| | Ca radial | 158.6 | | |
| | Mg | 52.6 | | |
| | Mg radial | 52.6 | 14.4 | |
| | S | 69.4 | 129.6 | |
| | Si | 9.3 | 15.7 | |
| Co Comp | Ca | 158.6 | 57.5 | 193.3 |
| | Ca radial | 158.6 | | |
| | Mg | 52.6 | | |
| | Mg radial | 52.6 | 12.7 | |
| | S | 69.4 | 109.9 | |
| | Si | 9.3 | 13.2 | |
| Zn Comp | Ca | 158.6 | 53.8 | 215.9 |
| | Ca radial | 158.6 | | |
| | Mg | 52.6 | | |
| | Mg radial | 52.6 | 16.4 | |
| | S | 69.4 | 130.3 | |
| | Si | 9.3 | 15.3 | |

Reagan Turley, Jose Hernandez Viezcas
(Gardea-Torresdey)

# Target Contaminants

| Sample | Methylene Blue | As (II),(V) | Pb (II) | Selenium | Naphthenic Acids |
|---|---|---|---|---|---|
| GO-BTC (Cu,Ni,Co,Zn) | | | | | |
| GO-BDC (Zr) | | | | | |
| GO-ZIF (Co, Zn) | | | | | |
| BNNS-BTC (Cu, Ni, Co,Zn) | | | | | |
| BNNS-ZIF (Co, Zn) | | | | | |
| AC-BTC (Cu, Ni, Co, Zn) | | | | | |
| AC-BDC (Zr) | | | | | |
| AC-ZIF (CO, Zn) | | | | | |



No removal

Efficient removal

Possible removal

# Acknowledgements

**UTEP**
- Karen Ventura
- Mariana Marcos
- Prof. Gardea-Torresdey

**Yale**
- Prof. Elimelech
- Dr. Tong
- Prof. Zimmerman
- Dr. Amanda Lounsbury

**RICE**
- Prof. Wong
- Camilah Powell

**RICE**
- Prof. Westerhoff
- Dr. Ariel Atkinson

**NMSU**
- Dr. Wang

**Undergraduate students**
- Roy Arrieta
- Jonathan Gracida
- Jerrin Philips

The University of Texas System

NEWT

NSF CHE-1305124

HHMI HOWARD HUGHES MEDICAL INSTITUTE

UTEP MINERS

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| 4:40 PM | Characterizing Wastewater Behavior of Titanium Dioxide Nanoparticles | Travis Waller |
| 5:10 PM | Facile Modification of Bi2WO6 with Base for Improved Photocatalytic Activity under Visible Light | Bangxing Ren |
| 5:30 PM | Quantitative Understanding of Nanoparticle Flocculation in Water Treatment | Sungmin Youn |