Layered structure of [Cu$_2$(bdc)$_2$(dabco)]$_n$-MOF shown from the [1 0 0] direction.

The research objectives were to design a 2D metal organic framework (MOF) nanosheets and their composites with high free-volume polymers that are functionalized with basic groups to increase the CO$_2$ solubility selectivity of the membrane. They employed computational modeling to gain predictive insight on the polymer/MOF, MOF/CO$_2$ and polymer-CO$_2$ interactions. In addition, mesoscale methods were used to quantify absorptions isotherms associated with CO$_2$/polymer, CO$_2$/MOF, and CO$_2$/composite membrane structures. These computational studies of CO$_2$ interactions with the materials were used to inform the experimental efforts so that composite membranes with optimized interactions with CO$_2$ will be synthesized. The champion composite samples from Penn State were compared against the literature and NETL’s state-of-the-art materials.
### Benefits:
The researchers have demonstrated the ability to successfully separate carbon dioxide from nitrogen using new mixed matrix membranes with 2D MOFs incorporated into polymer matrices. These systems were successfully modeled to gain insight into the molecular-level processes at work in these materials. They demonstrated key sights for modification to influence CO₂ sorption in MOFs. They also demonstrated mixed matrix membranes near the upper bound for CO₂/N₂ separations using their approach. Through this project, the researchers gained insights into promising materials for further development as gas separation membranes.

### Accomplishments:
In this project, the researchers accomplished the major goal of demonstrating the gas separation performance of mixed matrix membranes using cationic polymers and 2D (metal organic framework) MOF materials. These systems were successfully modeled to probe the molecular mechanisms at work in these materials that contribute to their gas separation performance properties. They demonstrated that the addition of 2D MOFs to polymer membranes can move the gas separation performance of the mixed matrix materials closer to the upper bound. This is a significant advancement and demonstrates the validity of their approach. While further optimization of these materials is needed for more gas separation membrane testing, this work points towards a promising direction for future work.

### NETL Collaboration:
Penn State had fruitful discussions with NETL on the state-of-the-art in modeling and experimental work in gas separation membranes. NETL was very helpful in describing their optimization pathway and the materials performance for different polymer/composite gas separation membranes.

### Relevant Publications: