U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

BIOENERGY TECHNOLOGIES OFFICE

BIOPROCESSING SEPARATIONS CONSORTIUM

Computational Studies Supporting Experimental Designs (Task 3.2)

BETO 2023 Project Peer Review

Performance-Advantaged Bioproducts and Bioprocessing Separations

April 6, 2023

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Project overview

Computational task helps experimental design of advanced bio-separation technologies

- Aims to strategize and accelerate material/process discovery and design in bio-separation processes.
- Helps development of technologies identified in three experimental tasks:

Task 2.4 Diol Separations

- Identify proper solvents for a cost-effective and scalable separation to recover 2,3-butanediol (BDO) from fermentation broth via solvent extraction.

Task 2.6 Enabling SAF Production by Adsorptive Denitrogenation (ADN)

- Find suitable regenerable sorbent materials for selective, deep nitrogen (N) removal from sustainable aviation fuel (SAF) by using ADN systems.

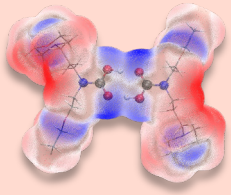
Task 2.7 Volatile Products Recovery

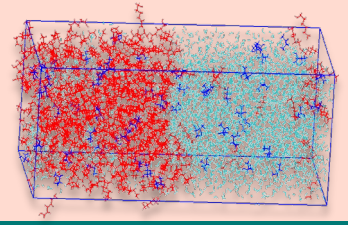
- Develop engineered adsorbents with tailored surface chemistries to passively capture products from bioreactor off-gases at larger scales/higher technical readiness levels.

Approach

Advanced data science bridges molecular-scale modeling and macroscopic experiments

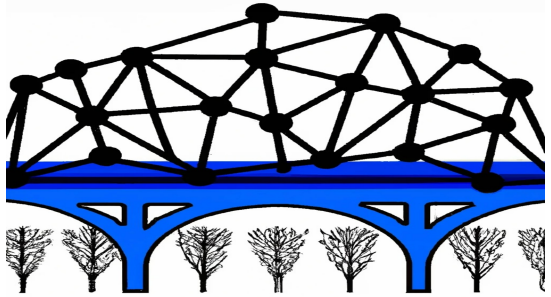
- Molecular modeling helps understand the underlying physics/chemistry features that govern the structure-property relationship in experimental measurements.
- Data science methods enhance the predictive power of molecular modeling by filling the gap between subatomic features and macroscale material properties.





Electronic structure
- Density functional theory
- Energy decomposition analysis

Statistical mechanics
- Classical molecular dynamics
- Enhanced sampling method



- Data analysis
- Machine learning
- Global optimization

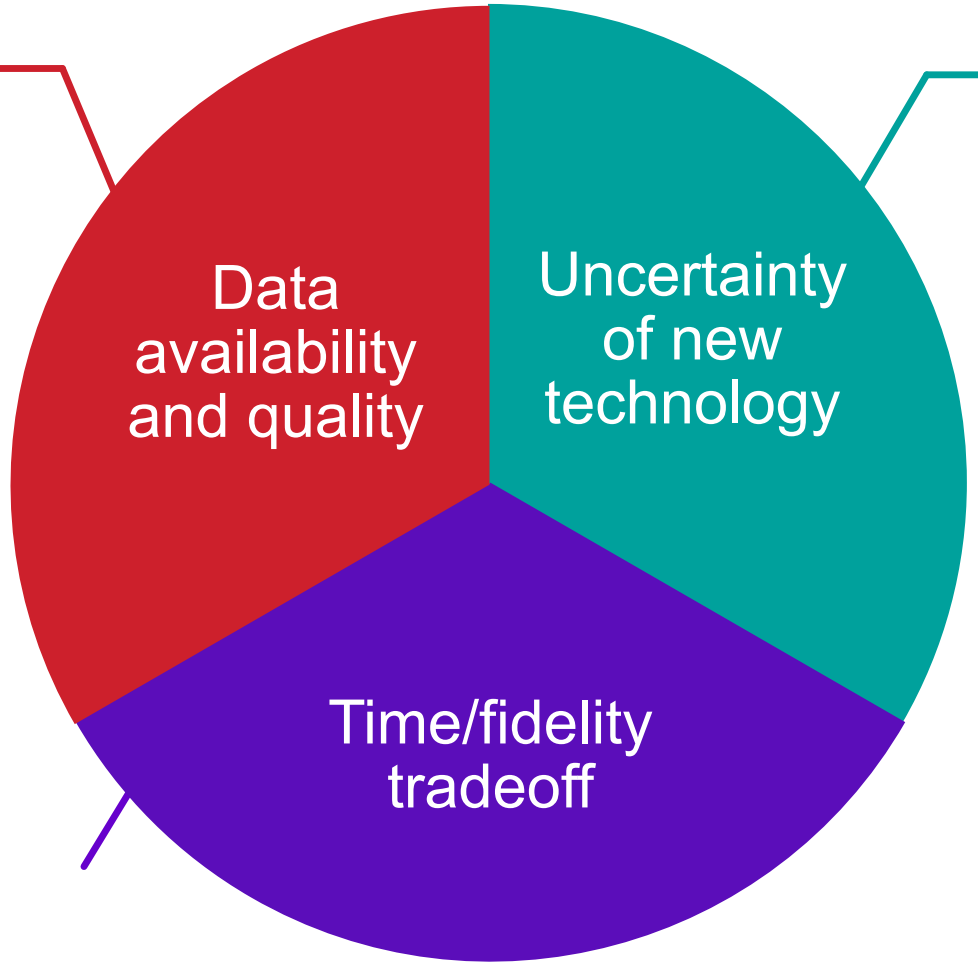
Experiments
- Property characterization
- Separation performance

Approach

We identified pathways to address challenges and mitigate risks

- Conduct key molecular calculations and simulations as needed.
- Active/transfer learning.

- Balance between accurate methods and fast methods in modeling.
- “Last mile” use of machine learning.

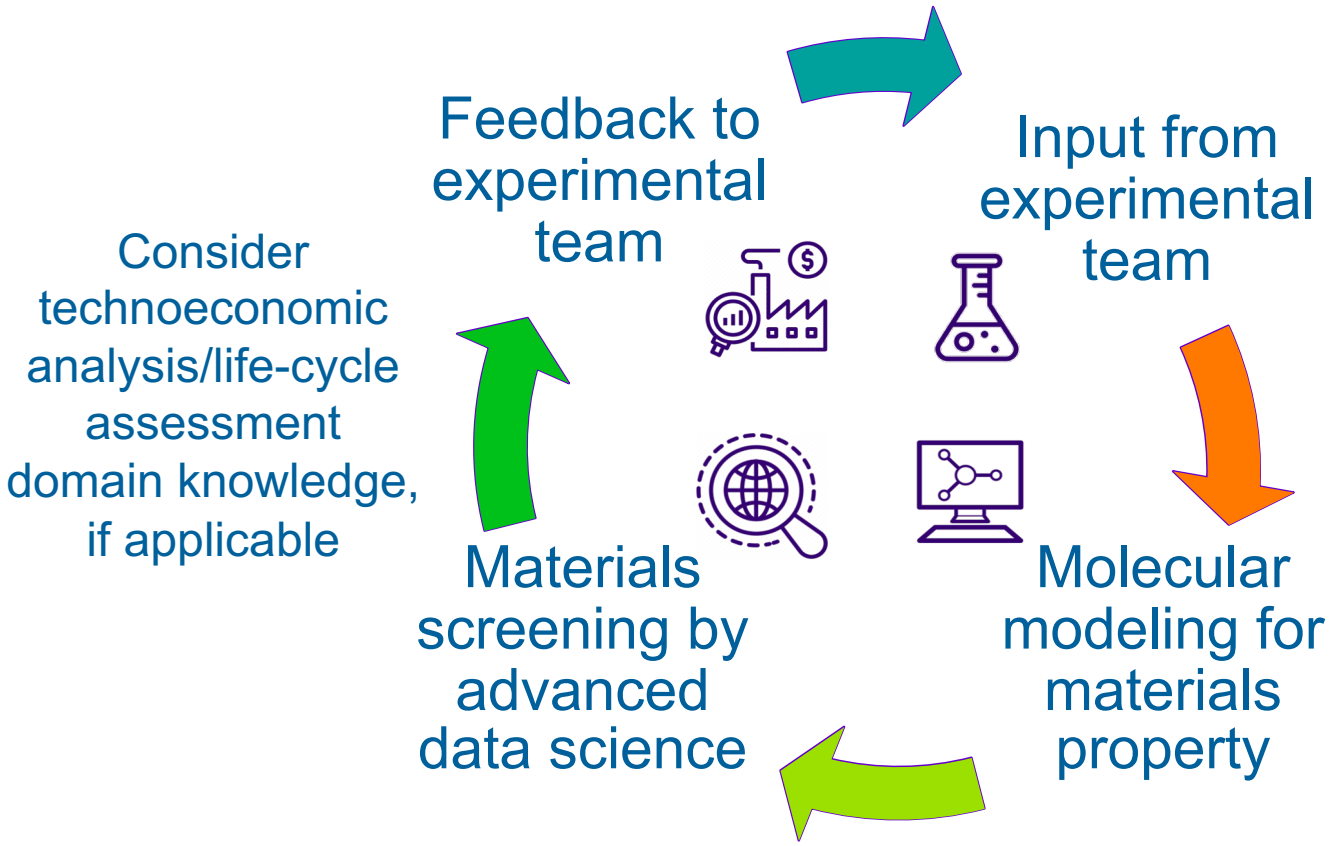


- Collaborate with other Bioenergy Technology Office projects, e.g., Consortium for Computational Physics and Chemistry (CCPC).
- Outreach for industrial partners with computation/ artificial intelligence expertise in bio-separation to join advisory board.

Diversity, Equity, and Inclusion activity: Contributed to topic development and supported student internship for the Bioenergy Bridge to Career Program.

Approach

Task management is facilitated by a collaborative recurring cycle with experimental teams.



- Regular meetings (biweekly/monthly) among different teams
- Documented progress:
  - Consortium FY23 Q2 milestone

Milestone Example	Task Detail	Due Date
Computationally screen potential volatile compounds that can be captured by xerogels in Task 2.7.	Identify at least two promising volatile compounds that are suitable for capture using xerogels based on evaluation of sorbent/sorbate interactions.	3/31/2023

Approach

Internal documented track of progress for technical metrics

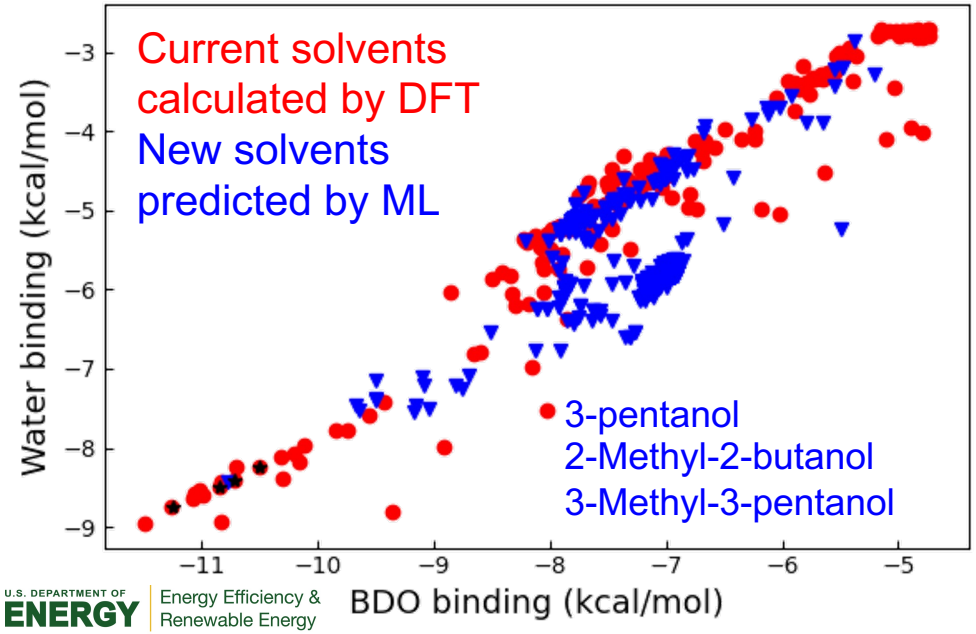
Task description	Status	Due date	Responsible lab
Task 2.7 Provide a list of industrially related volatile compounds (target 10 compounds) for computational screening.	100%	January 16, 2023	Argonne/PNNL
Task 2.6 Determine the list of functional groups to be computationally screened.	100%	January 31, 2023	PNNL/ORNL
Task 2.4 Finalize preliminary machine learning (ML) model to predict the partition coefficient of BDO/water in solvents.	100%	February 28, 2023	PNNL/ORNL
Task 2.7 Computational screening of compounds provided by experimental team by density functional theory (DFT)/semi-empirical/ML modeling.	80%	March 31, 2023	PNNL
Task 2.4 Discuss and identify desired properties of better solvents.	60%	April 30, 2023	PNNL/ORNL
Task 2.6 Computational screening of functional groups for their interaction with N-compounds, especially for non-basic compounds.	40%	May 31, 2023	PNNL
Task 2.6 Improve ML modeling and provide suggestions on sorbent candidates for ADN.	0%	July 31, 2023	PNNL/ORNL
Task 2.4 Screen solvents using ML modeling to predict the solubility of BDO/water in different solvents.	0%	September 30, 2023	PNNL/ORNL
Task 2.7 Improve ML modeling by considering transport property.	0%	September 30, 2023	PNNL

Progress and Outcomes – Task 2.4 Diol Separations

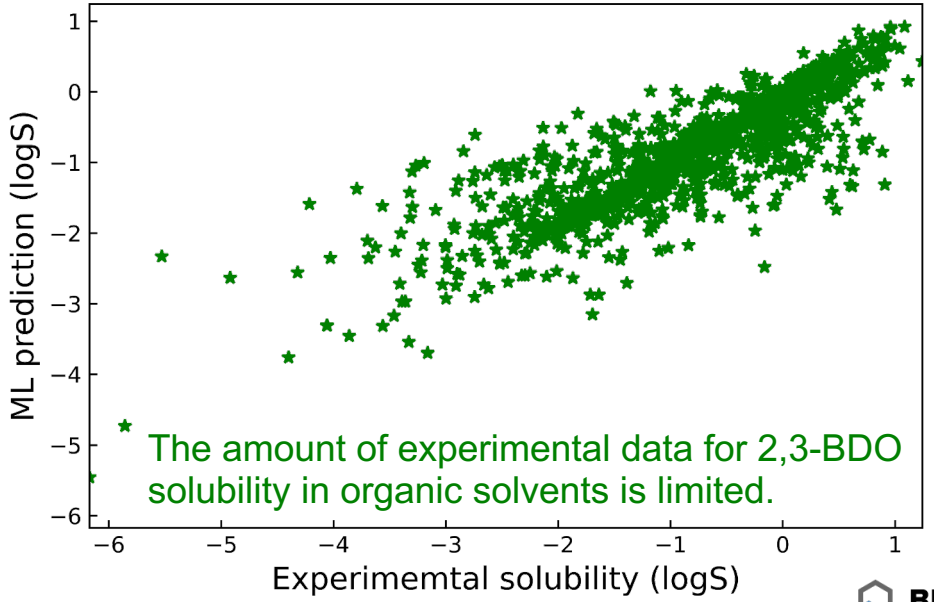
Predictive modeling expedites the search of proper solvents for solvent extraction of 2,3-butanediol

- A machine learning (ML) model, trained by 178 solvation energies from quantum chemistry modeling, was developed to screen >500 new solvents for 2,3-butanediol (2,3-BDO) extraction.
- Current focus on solubility prediction greatly accelerates the development of solvent extraction systems to separate 2,3-BDO from fermentation broth.

Solvation energy predicted by ML identifies promising solvent candidates.



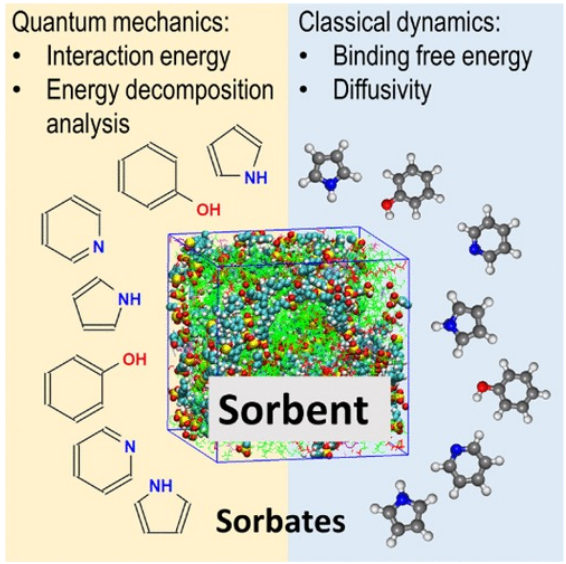
The ML prediction of solubility in organic solvents needs further improvement due to data availability.



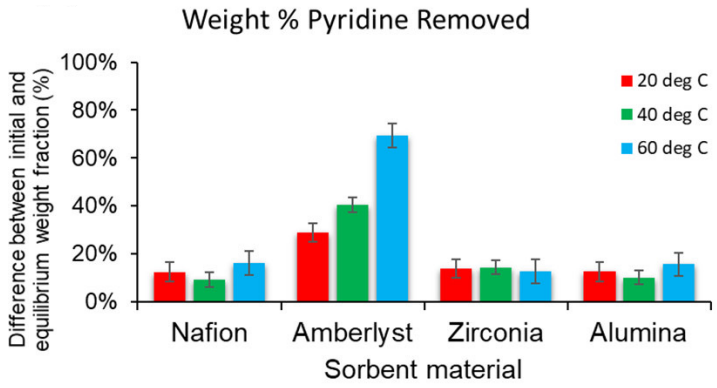
Progress and Outcomes – Task 2.6 Adsorptive Denitrogenation

Computational screening facilitates the development of regenerable sorbent materials to remove N compounds

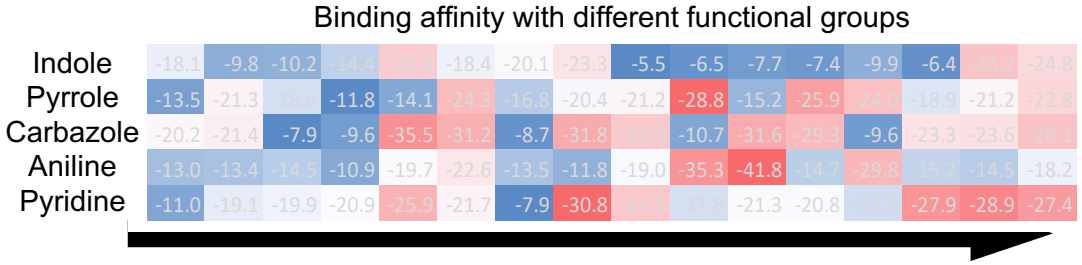
- Molecular modeling suggests that Amberlyst resin is a promising sorbent candidate for adsorptive denitrogenation of basic N compounds (e.g., pyridine).
- An effective screening is required to identify regenerable functionalities for the removal of both basic and non-basic N compounds (e.g., pyrrole, indole).



Molecular modeling of deep N removal



A principial component analysis reveals a possible correlation between the structure and binding strength of sorbent functionalities

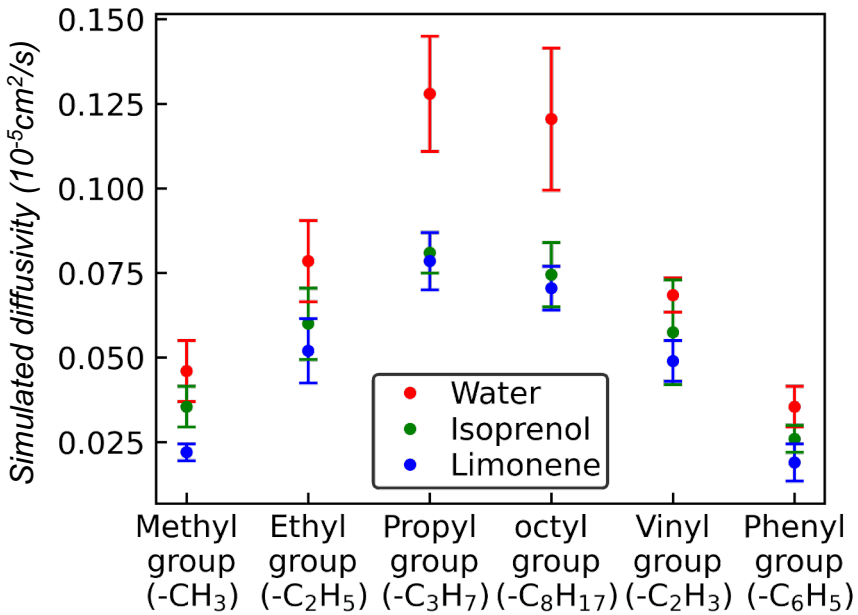


Principal component #1 contains structural features, e.g., topological polar surface area, fragments, molecular polarity, pKa)

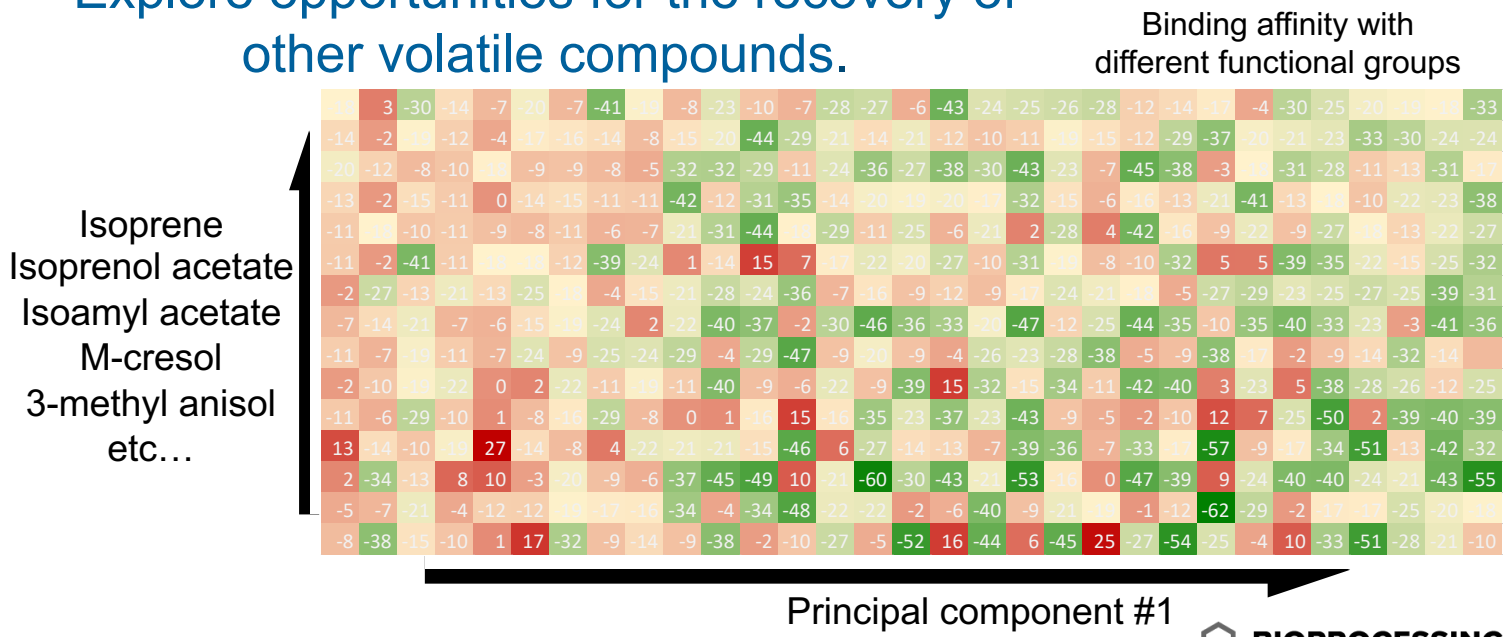
Progress and Outcomes – Task 2.7 Volatile Products Recovery

Molecular modeling guides the design of surface chemistry of xerogels to capture volatile compounds

- Our molecular modeling shows that long alkyl chains (>C3) on xerogel surfaces provide better separation capability for limonene and isoprenol.
- New research opportunities are identified via a computational screening of additional volatile compounds that could be recovered by tailored xerogels.



Explore opportunities for the recovery of other volatile compounds.

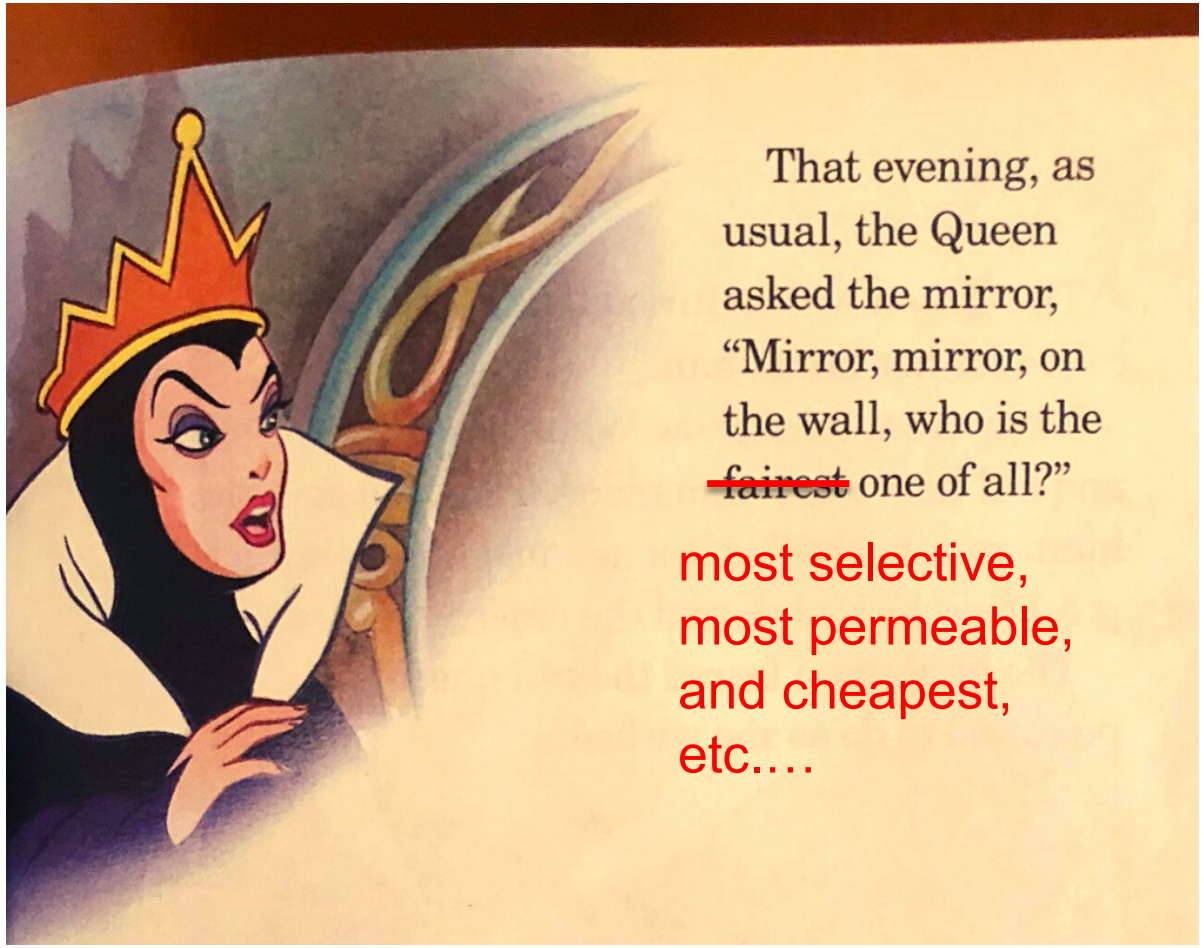


On track to meet FY23 Q2 milestone.

Impact

Computational modeling offers guidance to advance the materials discovery and process design

- Guides research teams in relevant experimental tasks to expedite development of new bio-separation technologies.
- Provides theoretical tools that are publicly available to resolve a broad range of bio-separation questions (e.g., solubility prediction in industry).
- Refer to experimental task for more industrial-relevant impact in detail.



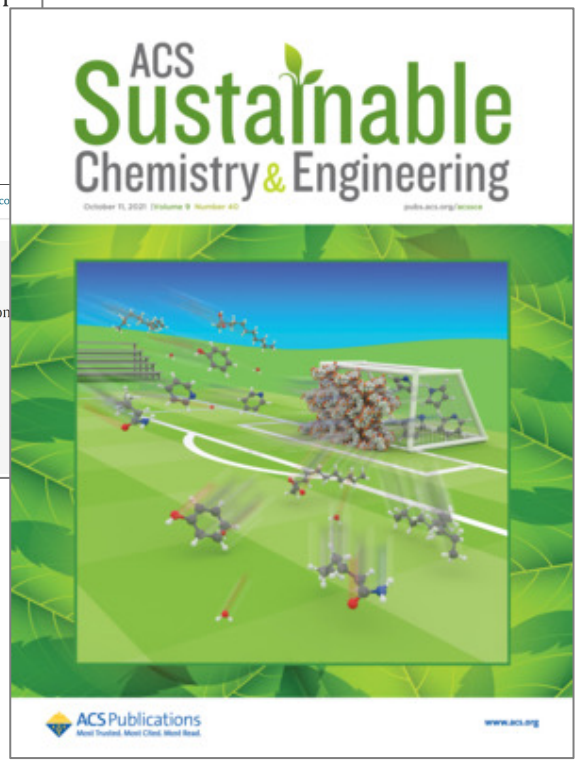
Impact

Integrating computational modeling explores new opportunities that align well with industrial interests.

- Pioneers new research opportunities and techniques for industrial/BETO interests, e.g., novel materials/process for decarbonization of transportation or industry.
- Industry feedback from American Chemical Society Green Chemistry and Engineering sessions and SepCon listening days supports the important role of integrating computational modeling into modern research and development.
- Disseminates accomplishments in high-impact journals.

J. Membr. Sci., IF=8.743

ACS Sustain. Chem. Eng., IF=9.224



Summary

- Computational task aims to guide experimental teams to accelerate and advance materials discovery and process design in bio-separation processes.
- Computational task currently works closely with experimental teams in three tasks: Task 2.4 Diol Separations, Task 2.6 Enabling SAF production by ADN, and Task 2.7 Volatile Products Recovery.
- Advanced data science technologies are applied to fill the gap between molecular modeling and experimental process.
- We developed/are developing predictive tools to enable computational screening that can be applied to a wider range of BETO-related applications.
- We will identify new research opportunities that align well with industrial/BETO interests using computational screening.

Quad Chart Overview

Timeline

- Project start date: October 2022
- Project end date: September 2025

	FY22 Costed	Total Award
DOE Funding	(10/01/2021 – 9/30/2022) $200K	(negotiated total federal share) $1.2M
Project Cost Share *	N/A	N/A

Project Goal

The computational task aims to develop a computational predictive tool, by integrating molecular modeling and ML, to guide experimental teams to (1) identify proper solvents for efficient solvent extraction of 2,3-BDO, (2) find suitable sorbents for selective deep N removal from SAF, and (3) develop xerogels with tailor surface groups for effective recovery of volatile compounds.

End of Project Milestone

Help supported experimental tasks be successful by identifying proper material candidates for each task. Develop predictive tools to enable computational screening that can be applied to a wider range of BETO-related applications.

TRL at Project Start: N/A
TRL at Project End: N/A

Project Partners

- ORNL, ANL, PNNL

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U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy
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- Malgorzata Makos

NERSC

Thank you!

Additional Slides

Publication, Patents, Presentations, Awards, and Commercialization

- Zhang, D., Gurunathan, P., Valentino, L., et al (2021). Atomic scale understanding of organic anion separations using ion-exchange resins. *Journal of Membrane Science*, 624, 118890.
- Gurunathan, P. K., Zhang, D., Glezakou, V. A., et al (2021). Computational and Experimental Study for the Denitrification of Biomass-Derived Hydrothermal Liquefaction Oil. *ACS Sustainable Chemistry & Engineering*, 9(40), 13406-13413.
- Zhang, D., Church, A. L., Kidder, M. K., et al (2022). Computational exploration of a sulfonated polybenzimidazole membrane for 2,3-butanediol/water separation. *Journal of Membrane Science*, In review.