Modeling a better catalyst for PIBSAs

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Polyisobutenyl succinic anhydrides (PIBSAs) are important for the auto industry because of their wide use in lubricant and fuel formulations. Their synthesis, however, requires high temperatures and, therefore, higher cost.

Adding a Lewis acid—a substance that can accept a pair of electrons—as a catalyst makes the PIBSA formation more efficient. But which Lewis acid? Despite the importance of PIBSAs in the industrial space, an easy way to screen these catalysts and predict their performance hasn't yet been developed.

New research led by the Computer-Aided Nano and Energy Lab (CANELa) at the University of Pittsburgh Swanson School of Engineering, in collaboration with the Lubrizol Corporation, addresses this problem by revealing the detailed mechanism of the Lewis acid-catalyzed reaction using computational modeling. The work, recently featured on the cover of the journal *Industrial & Engineering Chemistry* Research, builds a deeper understanding of the catalytic activity and creates a foundation for computationally screening catalysts in the future.

"PIBSAs are commonly synthesized through the reaction between maleic anhydride and polyisobutene. Adding Lewis acids makes the reaction faster and reduces the energy input required for PIBSA formation," explained Giannis Mpourmpakis, the Bicentennial Alumni Faculty Fellow and associate professor of chemical and petroleum engineering at Pitt. "But the reaction mechanism has not been well understood, and there are not many examples of this reaction in the literature. Our work helps to explain the way the reaction happens and identifies Lewis acids that will work best."

This new foundational information will aid in the discovery of Lewis acid catalysts for industrial chemical production at a faster rate and reduced cost.

"The alliance between the University of Pittsburgh and Lubrizol has been instrumental in demonstrating how Academia and the Chemical Process Industry can work together to produce commercially relevant

results," said Glenn Cormack, Global Process Innovation Manager at The Lubrizol Corporation. "Combining the knowledge and expertise of the Swanson School of Engineering and The Lubrizol Corporation allows both parties access to some of the best available computational and experimental techniques when exploring new challenges."

The research is one of many collaborations between Pitt and the Lubrizol Corporation, an Ohio-based specialty chemical provider for transportation, industrial and consumer markets. The alliance with Lubrizol, now in its seventh year, provides students with hands-on opportunities to experience how the knowledge and skills they're developing are used in the chemical industry. At the same time, students gain world-ready knowledge how Pitt's research helps improve Lubrizol's processes and products.

"Over the last few years, our partnership with Lubrizol has led to new, innovative ways for Lubrizol to make products and rethink their manufacturing processes," said Steven Little, William Kepler Whiteford Endowed Professor and chair of the Department of Chemical and Petroleum Engineering. "We learn a tremendous amount from them as well, and all of these publications are evidence of an alliance that continues to grow."

The paper, "Computational Screening of Lewis Acid Catalysts for the Ene Reaction between Maleic Anhydride and Polyisobutylene," was published in the ACS journal *I&EC Research*. It was authored by Cristian Morales-Rivera and Giannis Mpourmpakis at Pitt and Nico Proust and James Burrington at the Lubrizol Corporation.

More information: Cristian A. Morales-Rivera et al, Computational Screening of Lewis Acid Catalysts for the Ene Reaction between Maleic Anhydride and Polyisobutylene, *Industrial & Engineering Chemistry Research* (2020). DOI: 10.1021/acs.iecr.0c04860

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