Researchers make important discovery for 'smart' films and encapsulation

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Jonathan Whitmer, assistant professor in the Department of Chemical and Biomolecular Engineering and principal investigator for the study. Credit: Matt Cashore/University of Notre Dame

A study from the University of Notre Dame has found that the properties of a material commonly used to create conductive or protective films and encapsulate drug compounds—and the conditions in which this material will disassemble to release that medication—may be different than initially thought.

Published in the *Journal of the American Chemical Society*, the study aimed to identify the conditions under which polyelectrolyte complexes, or PECs, would assemble and stay assembled. The researchers found new, important differences between strong and weak PECs.

"The mechanism of weak PECs is completely different than that of strong PECs," said Jonathan Whitmer, assistant professor in the Department of Chemical and Biomolecular Engineering and principal investigator for the study. "During our research, we found that when each of the weak polyelectrolytes came together in a solution, the presence of an oppositely charged polymer resulted in a strong pKa shift, enabling both polyelectrolytes to become highly charged and to stay stable. On the contrary, pH has relatively little influence on the charge and assembly of strong PECs, whose strong binding to salt ions determines most of their assembly."

Weak PECs have been studied for many uses, including as a material to create capsules that hold medications. Weak PECs have a unique ability to bond and release in certain environments, but Whitmer's team found that pH affected the overall assembly of weak PECs, as well as the conditions in which these materials may release.

"This study completely changes our perspective on the formation of weak PECs and how this material can be used," said Whitmer, an affiliated member of NDnano. "Not only does this study point out physical mechanisms that will enable us to engineer better PECs, but it also has the potential to improve how this material can be utilized in industry, including the 'smart' encapsulation and delivery of medications, thin conductive materials and protective coatings."

In conducting the study, Whitmer and his team also developed a novel simulation algorithm. This algorithm allowed the researchers to analyze certain aspects of weak PECs that were not possible before, including the proper replication of solution conditions.

More information: Vikramjit S. Rathee et al, Role of Associative Charging in the Entropy–Energy Balance of Polyelectrolyte Complexes, *Journal of the American Chemical Society* (2018). DOI: 10.1021/jacs.8b08649

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