Manipulating a molecule's aversion to water gives scientists a building block for smart polymers

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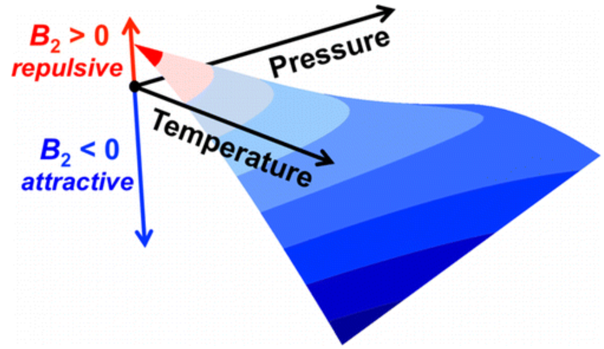

Graph of how methane molecules become more or less repelled from water as pressure and temperature changes.

Credit: Henry S. Ashbaugh, Tulane University.

Explanation: When you mix oil and water, you can see them separate right before your eyes. What you can't see is all of the interactions occurring at the molecular level. In the world of chemistry and physics, these interactions are of great interest.

How repelled a molecule is from water is called "hydrophobicity" and researchers at Tulane University in New Orleans, Louisiana are studying the fundamental physics behind hydrophobic interactions in order to develop smart polymers. Changing conditions like pH, temperature, light, or pressure can change the hydrophobicity of molecules within smart polymers in a way that is useful. For example, smart polymers can be designed to encapsulate a liquid medicine and release it after it travels through the body and reaches a targeted organ.

The research team is using supercomputers to simulate and analyze the hydrophobic interactions of molecules in water as different temperatures and pressures are applied. Computational research has tremendous advantages for discovery because it greatly speeds up testing times and the experiments can be conducted virtually.

Outcome: Hydrophobic interactions are so complicated that scientists have not been able to match theoretical calculations with actual lab experiments. However, the computational researchers at Tulane have brought us one step closer to understanding by successfully mapping methane molecule interactions in water over a wide range of states. This methane "map" is of the mathematical kind, known as a coefficient. It will allow the scientists to determine exactly what is occurring between molecules in both simulations and in physical experiments.

Impact/Benefit: Using this coefficient, custom experiments can be designed to determine the best ways to manufacture smart polymers in the size and shape they want while exhibiting the behaviors that are needed. There are endless possibilities for the use of smart polymers in medicine, industry, and environmental remediation.