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Computational modeling of self-healing biobased asphalt materials

At the dawn of artificial intelligence and self-driving laboratories for materials design, automated generation of unbiased atomistic models that capture the complexity of molecular fluids in a computationally efficient way is a persistent challenge. This lack of atomistic models is especially relevant for biobased oils and bitumen to be used in more resilient and sustainable roads. Pavements are majorly damaged by bitumen aging and fatigue cracking by traffic load. These issues can be mitigated by promoting asphalt self-healing mechanisms with encapsulated rejuvenators. These complex fluids are intrinsically challenging to model with molecular precision, given the large variety and complexity of organic molecules in its composition, which has hampered their bottom-up molecular design. To address this limitation, we have developed an author-agnostic computational framework to generate data-driven representative models of any complex mixture of organic molecules directly from Gas Chromatography-Mass Spectrometry (GCMS), thus reducing human biases in model creation and providing a platform for self-driven digital development of molecular organic fluids in self-healing infrastructure. Our method generates statistically representative molecular samples that simplify the complexity of the fluid in a limited group of molecules, while capturing the critical chemical features needed to describe the overall properties of the mixture. These models have been used to perform molecular dynamics simulations, and to predict reactivity and diffusion mechanisms in self-healing asphalt materials. The computational work is assisting the experimental development of rejuvenators that are encapsulated in biobased natural spores that completely heal a crack into an aged bitumen sample in 50 min.

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