Accelerating Chemical Formulation and Providing insights Using Computational Methods

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Formulation is a vital field of chemical research and development, responsible for the generation of consumer products from raw chemical constituents. The process of chemical formulation has rarely been the focus of computational chemistry efforts. Computational chemistry has instead been focused at the early stage screening and molecular design, where it has had a notable impact in the past decade. Our work begins to apply computational chemistry applications to problems pertinent to formulation chemistry.

Our work to date, has focused on the generation of reusable computational analogues of common experimental procedures. These computational experiments aim to provide predictions and insights to experimental formulation chemists, in an effort to help guide the best use of experimental resources.

We present, several examples of such computational experiments which utilize a simulation method known as Dissipative Particle Dynamics (DPD). These computational experiments span: predicting phase separations, simulating micellar aggregation and partition coefficient predictions. We also address the issue of suitable parameterization of these simulation methods. We apply a data driven parameterization, accelerated by the application of machine learning, prior to our simulations. This ensures we are representing the physics and chemistry of the systems as accurately as possible within the constraints of the simulations.

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