

VISCOSITY INDEX IMPROVERS FROM FIRST-PRINCIPLES IN-SILICO SCREENING

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ABSTRACT

Reducing fuel consumption and emissions in transportation has become a main challenge for society. One way to achieve this is by focusing on the reduction of friction between engine parts, to improve overall efficiency. To control the film thickness between the sliding surfaces in an engine, the main factor appears to be the viscosity of the lubricant and more generally its rheological behaviour as a function of temperature and pressure. Adjusting the viscosity of base oil lubricants can be achieved via Viscosity Index Improvers (VII). VIIs enable finer control of the viscosity as a function of temperature and pressure, e.g. by increasing overall viscosity at high temperature, to counteract the lower base oil viscosity without affecting the low temperature behaviour. Over the years, advancements in VIIs technology have been focused on either modifying chemistries or manipulating the structure and architecture of traditional VI polymers. The mechanisms behind the functionality of VI additives are still poorly understood and, therefore, the release of disruptive, innovating polymers is scarce and limited.

In this work, we propose a molecular modelling and simulation framework (Fig.1) for in-silico screening of VIIs. Our framework uses machine learning algorithms to predict novel polymer compositions and structures, based on fitness functions compounded from thermodynamic, chemical and viscoelastic properties obtained via hybrid first-principles based multiscale modelling. More specifically, this involves: a) systematic coarse-grained polymer structure and composition model building stage, b) a machine learning (ML) stage to evolve and determine the best performing structural and compositional (including polar groups) cues from the non-linearities in viscosity vs shear-rate, from a first-principles derived coarse-grain force field, c) a systematic atomistic to coarse-grain mapping scheme to determine the closest off-the-shelf polymer compositions that reproduce the coarse-grain models interactions, d) a characterization stage to determine the atomistic scale thermodynamic, chemical, viscoelastic and

rheological mechanisms that distinguish high performing VIIs, from our 1st principles reactive and polarizable molecular dynamics simulation methods, and e) an experimental validation stage to synthesize the best performing VIIs determined from the in-silico strategy, within the top-down optimization cycle.

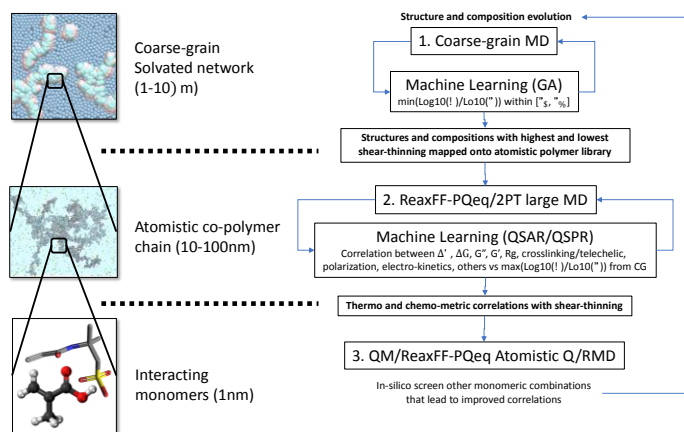


Fig.1 In-silico multiscale screening framework for development of enhanced VIIs, incorporates breakthrough technologies from the group at CALTECH including the reactive force field and molecular dynamics method ReaxFF[1], the polarizable force field PQeq[2], the 2PT method[3] for entropy and free-energy from short MD runs, the multi-objective ML framework [4], and others.

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