Speed-up lubricant formulation with computational chemistry tools

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ABSTRACT

Lubrication plays a major role in a wide range of key sectors such as automotive and industry. Renewal of lubricants is currently triggered by the quest of improved properties together with reduced environmental footprint. Molecular modeling is a powerful tool that already proven its ability in understanding reactivity of lubricant additives toward a surface [1-5] and combined with machine learning method, can screen candidates within defined physical-chemical properties [6]. An example will be presented in order to show how a fundamental study can be applied to an industrial issue and what will be the future challenge in computational chemistry.

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