Computational Screening of Soft Materials Systems with Application to Nano-Lubrication Systems

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Nanoscale devices featuring surfaces in sliding contact are subject to failure resulting from high surface area-to- volume ratios and high-energy surfaces that promote stiction and surface wear. Alkane-based monolayers have been proposed as a potential solution to these tribological issues, having been shown to reduce stiction while yielding low coefficients of friction. The tribological performance of monolayer lubricants is closely linked to their terminal group functionality, with, for example, group size, hydrophobicity, and hydrogen bonding shown to alter adhesion and frictional performance of monolayer films [1], [2]. Monolayer chemistry represents a vast parameter space, and thus a wide screening of various terminal group functionalities is desirable to obtain a thorough understanding of the links between chemistry and optimal tribological properties.

To this end, several tools recently developed in our group as part of the Molecular Simulation and Design Framework (MoSDeF) software suite [3], including the open-source mBuild [4], [5] and Foyer [6] packages, in conjunction with the Signac-flow workflow manager [7], have been designed to facilitate screening over such chemical/structural parameter spaces. In this work, we demonstrate the use of these tools to screen a pool of terminal group functionalities, spanning a wide chemical space, for optimal tribological properties. The effects on friction of various properties of the terminal group, such as hydrophobicity, aromaticity, and chemical family are analyzed, with relation to their influence on the underlying monolayer structure. Our work helps demonstrate how molecular screening can provide a framework for the design of better performing monolayer-based lubricants.

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