Friction and wear are the main source of failure for any kind of machinery. As technology scales down towards nano-mechanical systems, their detrimental effects can seriously hamper the functionality of these devices. Searching for appropriate lubricant is often a daunting task, due to the wide range of possible compounds, and the cost of performing the measurements. Predicting the performance of a lubricant could make the screening process of materials much faster and efficient, however, no simple model exists.

Machine-learning has been widely used in computer science and recently also for chemical and physical problems, such as the prediction of quantum mechanical properties of molecules [1]. We propose a method to machine-learn how the viscosity of liquids correlate to their molecular structure from experimental data. The fluid is described by a graph neural network [2], encoding the chemical bond structure of its molecules. This is used to compute a state vector of arbitrary size for the fluid, that is fed to conventional neural networks for calculation of density, viscosity and other properties simultaneously.