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Predicting high-pressure phase diagrams starting from the liquid

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We will present a methodology for predicting high-pressure phases of materials using molecular dynamics simulations of their compressed liquids as a starting point. The method combines first principles molecular dynamics simulations and such with machine learned potentials. It is aimed at predicting solid phases directly at elevated temperatures. We will show examples of its application and discuss its potential for addressing complex systems with impurities and nucleation.

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