Simulations of Liquid Metal Catalysts by molecular dynamics with Machine-Learned Force Fields

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Heterogeneous catalysis constitutes a vivid research area; a recently developed new concept is the usage of supported catalytically active liquid metal solutions (SCALMS). In SCALMS, a metal with a low melting point like gallium acts as solvent, in which the catalytically active atoms like platinum are dissolved at low concentration. When active atoms shortly arrive at the surface of the liquid, they act as isolated catalytic sites, since the gas phase reactants cannot enter the liquid metal. With this concept, the advantages of heterogeneous catalysis, easy product separation, are combined with those of homogeneous catalysis, well defined properties of isolated reaction sites.

The simulation of SCALMS, however, is a challenging task, due to the highly dynamical nature of the liquid metal. Direct ab-initio DFT molecular dynamics (MD) simulations are out of reach since several nanoseconds of molecular dynamics are needed for sufficient averaging. On the other hand, MD with conventional force fields lack the required accuracy. Moreover, in order to observe processes like the formation of intermetallic compounds or oxide layers, simulation cells containing several thousands of atoms are needed.

Machine-learned force fields (ML-FFs) are the method of choice to simulate SCALMS, since they do not rely on any preselected geometries or bonding situations, enabling the description of highly dynamical SCALMS. Their linear scaling with system size further enables the simulation of large time and length scales.

This poster presents how ML-FF simulations can be used in combination with electronic structure calculations to explain and predict trends in observed catalytic activities of different liquid metal catalysts. Furthermore, it features the real-time observation of fascinating phenomena like the formation of intermetallic phases.

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