Energy, Environmental, New materials

Development and application of data-driven simulation techniques for interface chemical processes

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Abstract

It is extremely important not only for fundamental points of view but also from application points of view to elucidate atomic structures, electronic properties, and chemical reaction processes at interfaces at the atomic level. Density functional theory (DFT) can calculate the atomic structures and electronic states at the atomic and molecular level with extremely high accuracy, but the calculations are very heavy, and the spatial and time scales of systems that can be handled are restricted to several nanometers, several tens of ps, respectively. On the other hand, by using empirical interatomic potentials, it is possible to elucidate phenomena with spatial sizes of sub μm and time scales of μs. By constructing machine-learned interatomic potentials that fit calculated results by DFT using state-of-the-art machine-learning techniques, larger-scale simulations with near-DFT accuracy become possible. In this research, we aim to elucidate various interfacial reactions using this method and to propose design principles or more desirable interfacial reactions.

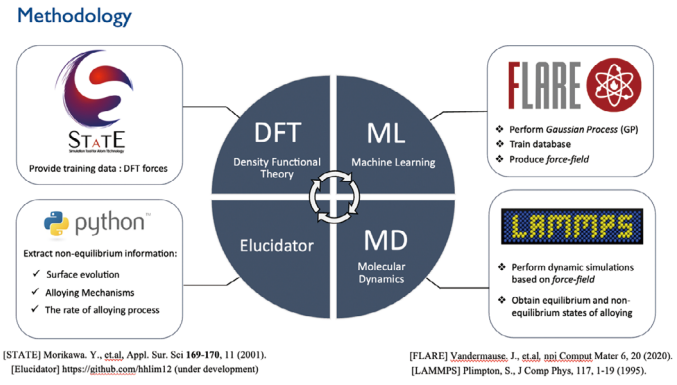
Background & Results

Highly accurate DFT calculations have played an extremely important role, but calculations are very heavy, so even with the latest supercomputers, it is necessary to use models with limited assumptions. Recent advances in machine learning methods have made it possible to derive highly accurate interatomic potentials from the results of DFT calculations for various structures. Interfacial reactions can be simulated under a more realistic device environment, and it is expected that in the future it will be possible to predict reaction processes and to design more desirable materials.

Significance of the research and Future perspective

Elucidating atomic structures, electronic properties, and chemical reaction processes at gas/solid, liquid/solid, or solid/solid interfaces at the atomic level is very important not only from fundamental scientific points of view, but is also useful for various applications such as heterogeneous catalysts, semiconductor devices, crystal growth, etching, fuel cells, secondary batteries, wear, and lubrication. However, it is often difficult to elucidate them experimentally. Therefore, elucidation at the atomic level by DFT calculations with high accuracy plays an extremely important role. However, due to the huge amount of calculations, the spatial scale of the system that can be calculated was limited to several nanometers, and the time scale was limited to several tens of ps. By fitting the DFT calculation results to the atomic force potential using state-of-the-art machine learning techniques, we are able to perform highly accurate calculations very quickly. By using this tequnique, we have clarified Cu-Zn surface alloying process, which are important in catalytic methanol synthesis. We clarified the elementary processes of the alloy formation by performing molecular dynamics simulations with space scales of sub-μm and time scales of μs using machine learning potentials. As a result, it was clarified that alloying progresses due to frequent exchange of atoms between the upper and lower step edge atoms near the atomic steps on the solid surface. This is qualitatively consistent with experimental observations using STM, but reveals that atomic processes frequently occurring are quite different from the experimentally proposed alloy formation. In this way, simulations based on machine learning potentials are extremely effective in elucidating elementary processes at the interface at the atomic level.

We will apply this effective method to various systems such as the surface oxidation etching process of diamond, which is important as a material for cutting tools and is expected to be a next-generation semiconductor for power and quantum devices, as well as other important catalysts and fuel cell electrode reaction processes.



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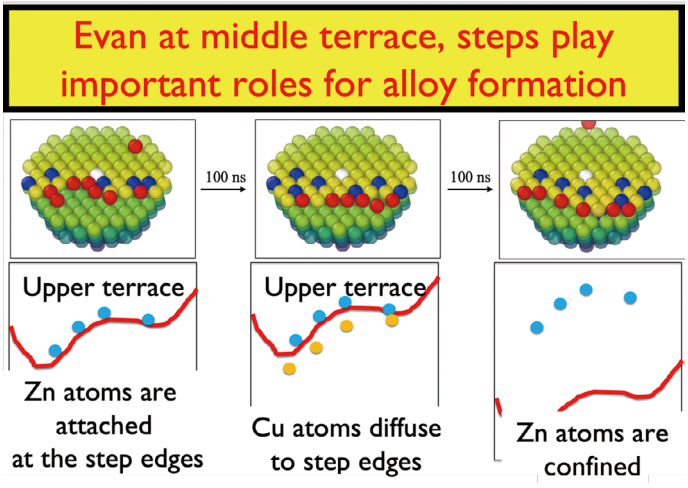

Patent

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Keyword density functional theory, machine learning, surface science, heterogeneous catalysis, electrochemistry