Oxidation and Hydrogenation of Monolayer MoS$_2$ with Compositing Agent under Environmental Exposure: The ReaxFF Mo/Ti/Au/O/S/H Force Field Development and Applications

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An atomistic modeling tool is essential to an in-depth understanding upon surface reactions of transition metal dichalcogenides (TMDs), such as molybdenum disulfide (MoS$_2$), with the presence of compositing agents, including Ti and Au, under different environmental exposures. We report a new ReaxFF reactive force field parameter set for Mo, Ti, Au, O, S, and H interactions. We apply the force field in a series of molecular dynamics (MD) simulations to unravel the impact of the Ti dopant on the oxidation/hydrogenation behaviors of MoS$_2$ surface.

The simulation results reveal that, in the absence of Ti clusters, the MoS$_2$ surface is ruptured and oxidized at elevated temperatures through a process of adsorption followed by dissociation of the O$_2$ molecules on the MoS$_2$ surface during the temperature ramp. When the MoS$_2$ surface is exposed to H$_2$O molecules, surface hydrogenation is most favored, followed by oxidation, then hydroxylation. The introduction of Ti clusters to the systems mitigates the oxidation/hydrogenation of MoS$_2$ at a low or intermediate temperature by capturing the O$_2$/H$_2$O molecules and locking the O/H-related radicals inside the clusters. However, OH$^-$ and H$_3$O$^+$ are emitted from the Ti clusters in the H$_2$O environment as temperature rises, and the accelerating hydrogenation of MoS$_2$ is consequently observed at an ultra-high temperature. These findings indicate an important but complex role of Ti dopants in mitigating the oxidation and hydrogenation of MoS$_2$ under different environmental exposures. The possible mechanisms of oxidation and hydrogenation revealed by MD simulations can give an insight to the design of oxidation resistant TMDs and can be useful to the optical, electronic, magnetic, catalytic, and energy harvesting industries.