Tribochemical Phenomena at Diamond-Silica Interfaces by Ab Initio and Machine Learning Molecular Dynamics

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Abstract

The diamond-silica interface is a system of high relevance for the chemical mechanical polishing of diamond and other technological applications. It can be also seen as a reference platform for assessing the behavior of diamond in terms of friction and wear under tribological conditions. We employ ab initio and machine learning molecular dynamics calculations for evaluating the impact of different diamond surface terminations and orientations, along with boron (B) doping, on the tribologically-induced interactions at the diamond-silica sliding interface. The Pandey-reconstructed C(111) surface behavior is found to be dominated by weaker van der Waals interactions and Pauli repulsion at the interface in all cases, while the C(110) surface is the most prone to wear. Among the different passivating species considered, F and H+OH terminations are the most efficient means of reducing friction and increasing interfacial separations. On the other hand, B dopants at the diamond surfaces are able to promote chemical interactions at the interface and more prone to be detached to silica. The study of large systems on the nanosecond timescale with quantum accuracy is made possible thanks to a workflow for smart configuration sampling (SCS) in active learning that permit to obtain machine learning interatomic potentials that are enough robust and accurate also in the characteristic harsh conditions generated by high loads and shear rates.
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