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# Advances in Atomic-Scale Tribological Mechanisms of Solid Interfaces

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**Abstract:** It is important to explain the tribological mechanism of solid interfaces at the atomic scale. Theoretical models developments involving atomic-scale tribology and the most classical first-principles theory for atomic-scale friction have been described. The construction of potential energy surface based on first-principle calculation is found extremely useful to unveil the tribological mechanism for atomic-scale solid sheets. Furthermore, atomic-scale tribological mechanisms exploring achievements for metals interfaces, tribo-chemistry, carbon-based solid lubrication material and 2H-MoS<sub>2</sub> have also been reviewed.

**Keywords:** Solid-solid Interfaces; Atomic-scale friction; First principle calculation; Molecular dynamic simulation.

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