
Monitoring the in situ formation of slippery tribofilms by ab initio and machine learning molecular dynamics

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Abstract

I will present the results of ab initio and machine learning molecular dynamics simulations that show how slippery layered materials can be synthesized at the tribological interface thanks to tribochemical reactions. In particular, I will show that selenide layers can be formed by sprinkling Se nanopowders onto sliding contacts (1) and graphene can be obtained by the tribologically-induced polymerization of aromatic molecules (2). Finally, I will discuss the potentiality of machine-learning interaction potentials to design self-assembled monolayers as friction modifiers (3).

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(3) H.T.T. Ta, M. Ferrario, S. Loehlé, and M.C. Righi, *Computational Materials Today*, 1 1000005 (2024)

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