Abstract #426 | Invited

When Surfaces Meet: Challenges in Computational and Experimental Coating Tribology

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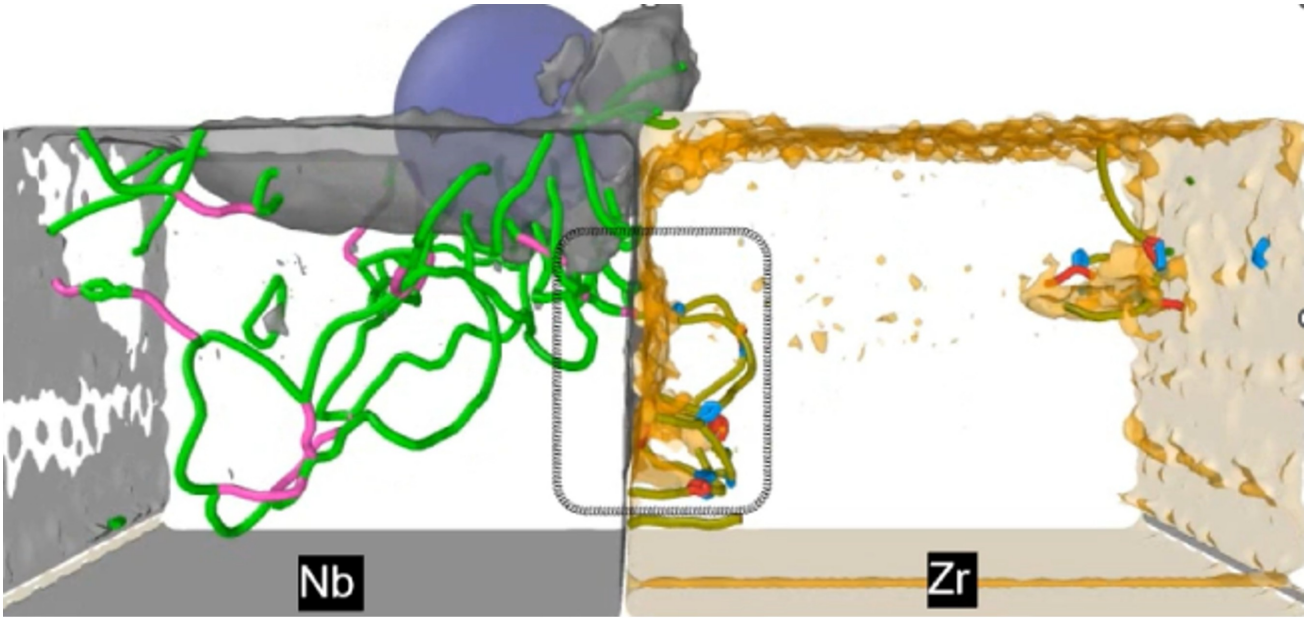
Computational materials science has opened fundamentally new routes for the design of functional surfaces and coatings. The assessment of thermal stability and phase transformations in highly complex compounds is now a relatively straightforward task, and the screening of millions of molecules to identify candidates with targeted properties has become routine. Mechanical response, sensing functionality, oxidation and corrosion resistance, and optoelectronic behavior are increasingly accessible through advanced atomistic simulations, often combined with machine-learning and neural-network approaches.

The potential of computational tribology has been recognized for more than two decades. Yet, despite remarkable progress in modeling tools and computational power, the reliable prediction of friction—particularly when sliding is accompanied by wear—remains an open challenge. Multiscale simulation strategies that have proven transformative in many other areas of materials science are still difficult to implement, even for nominally simple surfaces in sliding contact.

In this plenary lecture, we examine the central challenges of coating tribology from a materials-design perspective, with a particular emphasis on dry sliding, which is often more complex and less understood than fully lubricated contact. We begin by discussing how friction and wear are defined across different length and time scales, and by addressing the availability—and, more critically, the absence—of experimental data needed to inform and validate atomistic and higher-scale simulations. Drawing on examples from engineering practice, including sliding of ubiquitous carbon-based films, solid lubricants, and metallic coatings, we highlight recent advances in computational tribology and clarify their current limitations. Finally, we identify the key roadblocks that hinder bottom-up, predictive design of tribological coatings and outline possible pathways toward overcoming them.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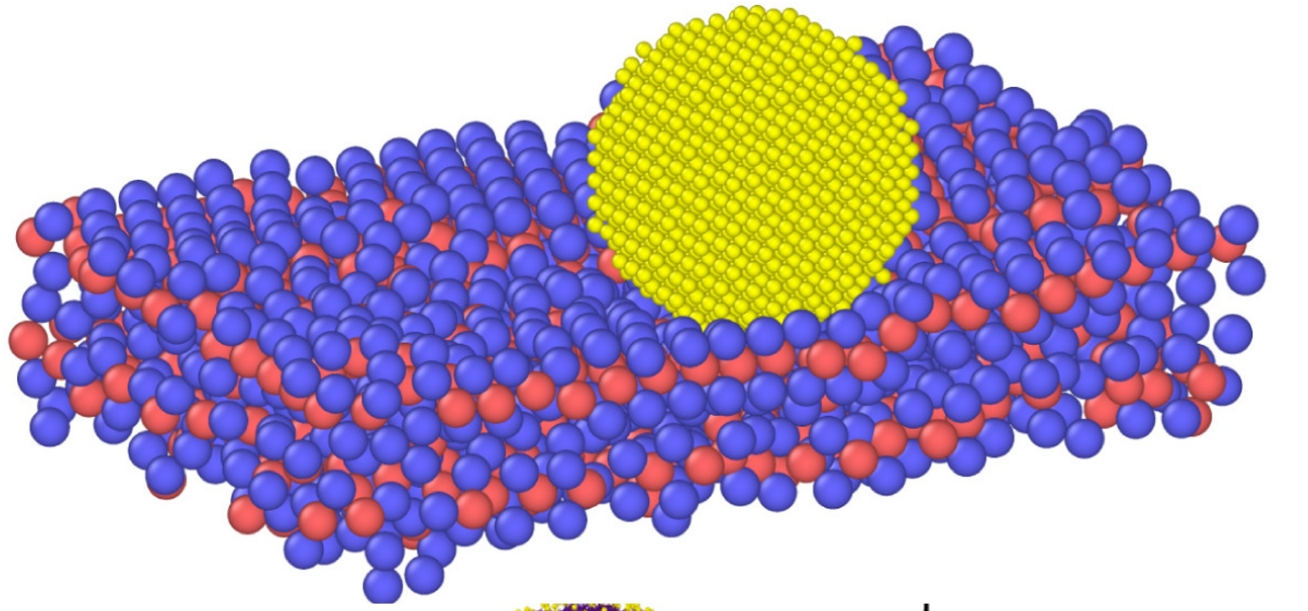

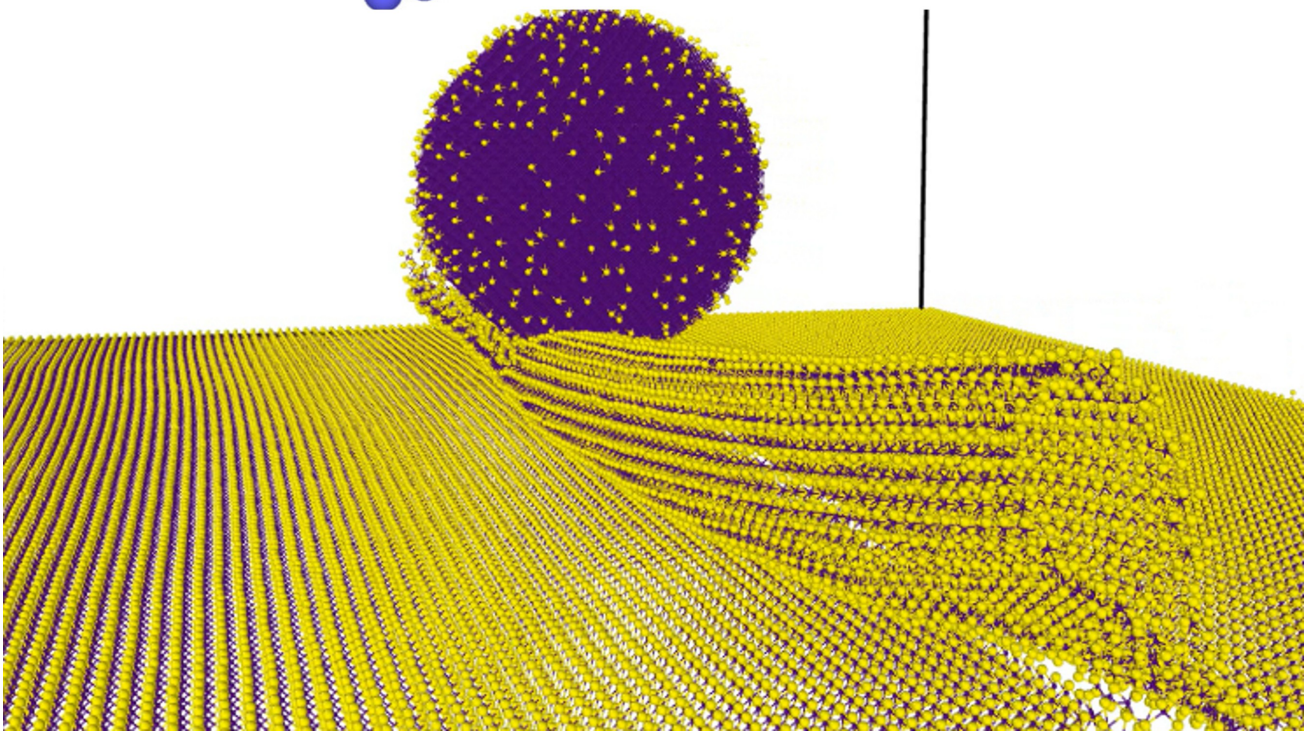

Molecular dynamics simulations of sliding
Nanoscale wear across the metallic interface, sliding of polycrystalline solid lubricant, and breakage of two-dimensional wrinkles.