

# **Toward Computational Design of Tribological Interfaces: Molecular Understanding of Friction, Adhesion, and Wear**

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## **Abstract**

Friction and wear are encountered in most mechanical contacts, but these properties become particularly important when specimen dimensions are scaled down to the nanoscale where the surface to volume ratio is high. Design of wear-resistant materials is currently hindered by our limited understanding of fundamental relationships between material's the nano/microstructure, surface chemistry and the measured friction. To provide such understanding, my group develops tools and carries out simulations that range from *ab initio* calculations to large-scale molecular dynamics to phase field simulations. In this talk I will discuss a few examples that include (i) chemical origins of time-dependent adhesion in silica contacts, (ii) size-effects in friction and wear as well as new frictional phenomena that emerge in nanocrystalline materials, and (iii) our developments of new tools for studies of friction and slip at liquid/solid interfaces.