Slipping and Sliding: First-Principles Simulations of Tribological Processes

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Friction and wear are ubiquitous phenomena that have significant environmental and economic impacts. For example, the annual costs associated with energy losses due to friction and the need to prematurely replace worn out equipment are estimated to be several percent of the GDP in industrialized nations. Furthermore, energy losses due to friction place additional demands on finite energy resources. In order to more effectively control friction and wear, it is necessary to have a better understanding of the processes that occur in sliding contacts. First-principles chemical simulation can play a key role in this respect, offering insight into the details of these processes at the atomic and electronic levels, and providing a means of characterizing the extreme conditions experienced in sliding contacts.

In this presentation, I will discuss our efforts to understand friction and wear through first-principles molecular dynamics simulations. Emphasis will be placed on two areas. First, I will discuss our ongoing efforts to develop models that relate friction forces and friction coefficients to measurable properties of sliding interfaces. The development of such models represents a significant advancement in the basic understanding of friction, with potential applications in many areas. Second, I will discuss work aimed at using the extreme conditions experienced in sliding contacts to transform simple molecules into effective lubricants. Specifically, I will show how compression and shear can transform simple molecules into oligomers, which can functional as lubricants. We suggest that reactions of this type could form the basis of a new approach to lubrication in which lubricant molecules actively adapt to the conditions experienced in contacts instead of merely acting as passive mechanical boundaries between sliding surfaces.