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Accurate multiscale simulation of frictional interfaces by Quantum Mechanics/Green's Function molecular dynamics

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We present an advanced multiscale approach based on linked quantum mechanics and Green's function molecular dynamics, which provides an accurate description of both the interface chemistry and the elastic properties of two semi-infinite bulks in contact. By considering a prototypical system composed by two diamond surfaces with different degree of passivation, we show that the presented method can be used not only for executing realistic in silico experiments of tribology, but also for uncovering fundamental aspects of the friction laws.

Keywords: Green's function, interfaces, molecular dynamics, multiscale simulations, tribology

1. Introduction

Ab initio molecular dynamics (AIMD) simulations provide a reliable description of the chemical interactions at the sliding interface but cannot be used to obtain quantitative estimates of the energy dissipation by phonons because of the use of slabs of finite thickness. Green's function MD (GFMD) constitutes an elegant way to overcome these limitations because it implicitly includes the influence of the infinite bulk atoms on the dynamics of surface atoms [1, 2]. The projection of the semi-infinite degrees of freedom allows representing the phonon energy dissipation and thermo/baro-stats in a well-defined manner [3]. Here we present an innovative procedure to link GFMD to AIMD, realizing a hybrid model able to describe the reactive friction interface with the high accuracy of quantum mechanics and at the same time include the proper control of temperature, mechanical stresses, and energy dissipation in non-equilibrium conditions.

2. Methods

The hybrid QM/GFMD scheme and its application to a prototypical tribochemistry system are shown in Figure 1. The two semi-infinite bulks are described by a collection of an infinite number of harmonic oscillators of first-principles derived spring constants. Their effect is fully taken into account by Green's function atoms, which are linked to the QM region. We adopted this scheme to study the sliding interface between two H-terminated diamond surfaces with different degrees of passivation [4].

3. Discussion

By employing our hybrid scheme, we analyzed the kinetic friction of two diamond semi-infinite bulks in contact. The friction coefficient and the interface morphology depend on the degree of passivation of the diamond surfaces, with superlubric regimes at high H coverages. The friction coefficient is very sensitive to the degree of surface passivation and increases with the number of unsaturated carbon bonds dangling at the surface. The simulations also highlight the difference between the static and kinetic tribological properties. We observe that the path followed by the system during sliding in non-equilibrium conditions deviates considerably from the minimum energy path. Furthermore, the kinetic friction force is much smaller than the static friction force due to the collective effects in the many-particle system.

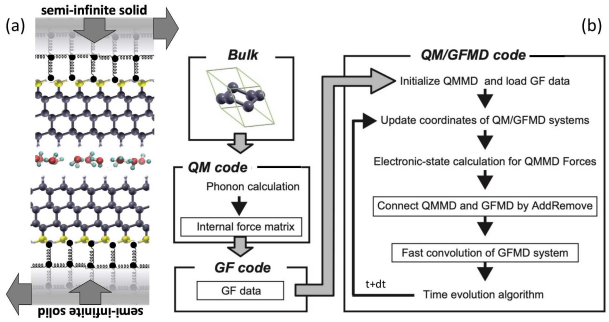

Figure 1: Representation of a solid-solid interface described by the QM/GFMD hybrid scheme (a) and a scheme developed QM/GFMD workflow (b).

4. References

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