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"Brownian motion near interfaces: Insights from μs-long molecular dynamics"

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(in collaboration with Prof. Izabela Szlufarska)

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When:	**Monday, March 2nd, 2015 3:30 pm**
Where:	**Room 1153 Mechanical Engineering Building**
Host:	**Prof. Izabela Szlufarska, MS&E Department**

ABSTRACT:
Near-boundary Brownian motion is a classic hydrodynamic problem of great importance in a variety of fields from biophysics to micro-/nanofluidics. However, due to challenges in experimental measurements of near-boundary dynamics, the impact of interfaces on nearby Brownian motion remains a highly debated topic. In this seminar, we will present insights into the effects of interfaces on Brownian motion obtained based on μs-long large-scale molecular dynamics simulations and our newly developed Green-Kubo relation for friction at the liquid-solid interface. We will briefly review the modern understanding of Brownian motion that explains the famous $t^{-3/2}$ long-time tail in the velocity autocorrelation function of a Brownian particle in bulk liquid, where t represents time. We will demonstrate that, near an interface, the long-time tail behavior changes to the $t^{-5/2}$ decay. We will discuss the limitations of classical assumptions of the hydrodynamic theories, such as the lack of slip at the solid/liquid interface and we will demonstrate that the presence of interfacial slip has profound effects on the nearby Brownian motion. Our results highlight the importance of accounting for liquid relaxation near interfaces in the hydrodynamic theories and in modeling of micro-/nano-flows, and they demonstrate the potential of Brownian-particle based sensors to probe the local wettability of liquid-solid interfaces.