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Fluids at an electrostatically active surface: Optimum in interfacial friction and hydroelectronic drag

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Fluids at solid interfaces are central to key technologies in energy conversion, electrochemistry, and catalysis, yet their nanoscale dynamics remain only partially understood. On metallic surfaces, recent studies have revealed unconventional interfacial phenomena—including complex electrostatic screening, anomalous wetting behavior, and quantum friction—that call for new modeling tools bridging charge dynamics in the metal with molecular motion in the fluid. In this work, we introduce a molecular simulation framework based on Virtual Thomas-Fermi fluids, enabling a realistic, atomically-resolved treatment of interfacial transport that captures both charge relaxation in the metal and its coupling to the surrounding liquid. Applying this approach to water near metallic surfaces with tunable screening properties, we uncover a non-monotonic dependence of interfacial friction on metallicity, peaking when charge relaxation modes in the solid and fluid dynamically overlap. Furthermore, we report a direct observation of hydroelectronic drag, a momentum transfer mechanism rooted in dynamic electrostatic interactions at the interface. These results shed new light on interfacial transport under electrostatic coupling and open avenues for designing metal–fluid interfaces with tailored frictional properties. We further discuss how these predictions could be directly tested via inelastic neutron scattering experiments targeting interfacial charge–density correlations.

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