

Sliding friction over individual covalent bonds correlates with bond order

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Unveiling the dynamics and energy dissipation involved in atomic scale motion is key to understanding surface catalysis, molecular motors, and single molecule manipulation. Despite significant progress in nanoscale friction studies, due to challenges in atomistically defining the sliding surfaces, there are outstanding problems regarding reproducibility, isolating nonconservative interactions, and in general reconciling atomistic theory with experimental results. This has prompted investigations with precise control at the single atom scale. We use a single atom asperity as one sliding surface. High spatial resolution allows us to investigate individual chemical bonds and address the question of how the nature of a chemical bond affects sliding friction. Surprisingly, we find a large variety in sliding friction over covalent bonds. Density functional theory-based simulations yield excellent agreement with the data and reveal that sliding friction is correlated to bond order. Finally, we show that over hydrogen bonds, the maximum magnitude of sliding friction can be similar to friction over covalent bonds, however that interaction is not with a bond (increased electron density between the atoms). These findings offer new insights into atomic-scale motion and show that the frictional properties of advanced materials and nanodevices can be tuned by selecting the nature and order of chemical bonds at surfaces.

Reference

[1] S. Nam, L. Hörmann, O. Gretz et al. PREPRINT (Version 1) available at Research Square [<https://doi.org/10.21203/rs.3.rs-6127312/v1>] (2025)