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Probing van der Waals Forces at the Single-Molecule Level

LATHA VENKATARAMAN, Columbia University

Single molecule junctions represent an attractive platform to understand and control functionality of materials and devices at the nanoscale. While their electronic transport properties have received tremendous attention thus far, measurements of mechanics are new and allow for a more complete understanding of the structure-function relationship of these atomic scale devices. Here we report simultaneous measurement of force and electrical conductance across Au-Bipyridine-Au junctions using a conducting atomic force microscope (AFM). We show that these junctions have two distinct structures each with a characteristic conductance. Using statistically relevant analysis, these two structures are found to have very different mechanical properties. Specifically, we find that the higher conductance junctions have a significantly larger rupture force and stiffness than the lower conducting junctions. They also have a larger rupture force than Au single-atom point contacts, suggesting multiple points of contact. Using density functional theory simulations we show that van der Waals (vdW) interactions between the pyridine ring and Au electrodes plays a key role in the junction mechanics. These measurements thus provide a quantitative characterization of vdW interactions at metal/organic interfaces at the single-molecule level [1].

[1] Aradhya, S. V., Frei, M., Hybertsen, M. S. & Venkataraman, L., Nature Materials, 11, 872-876 (2012).