Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Simultaneous conductance and mechanical measurements on single molecule junctions reveal enhanced binding due to van der Waals interactions[1] SRIHARSHA V. ARADHYA, MICHAEL FREI, Columbia University, MARK S. HYBERTSEN, Brookhaven National Laboratory, LATHA VENKATARAMAN, Columbia University — Quantitative measurement of Van der Waals (vdW) interactions at the single molecule level remains challenging in experiments and its accurate inclusion in first principles theory is also complex. Here we report simultaneous measurement of force and electrical conductance across Au-molecule-Au junctions using a conducting atomic force microscope (AFM) for 4,4'-bipyridine (BP) and 1,2-bis(4-pyridyl)ethylene (BPE) molecules. For each of these molecules two distinct molecular junction structures are observed with characteristic conductances, consistent with previous studies utilizing scanning tunneling microscopy (STM). 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 those that show the lower conductance. They also have a larger rupture force than Au point contacts, suggesting multiple points of contact. Density functional theory (DFT) calculations suggest that the rupture force for the low conductance structure is well characterized as arising from N-Au donor acceptor interaction. However, the large rupture force and stiffness of the high conductance structure is most naturally explained as being due to the vdW contributions.

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[1]Support: NSF CHE 07-44185 and The Packard Foundation

Date submitted: 07 Nov 2011 Electronic form version 1.4