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Simulation and Measurement of Single Molecule Junction Evolution Under Stress: Comparison of Amine and Phosphine Link Groups MAX KOENTOPP, Columbia University, MARK HYBERTSEN, Brookhaven National Laboratory, MARIA KAMENETSKA, ADAM WHALLEY, YOUNG PARK, MICHAEL STEIGERWALD, COLIN NUCKOLLS, LATHA VENKATARAMAN, Columbia University — Reliable measurements of single molecule conductance are performed by repeated breaking of Au point contacts in a solution containing target molecules with link groups that readily form donor-acceptor bonds to specific Au atoms on the electrodes. Measured traces present the junction conductance as a continuous function of junction elongation under applied stress. Our extensive experimental database shows strong correlation between measured conductance step length and molecular backbone length, with phosphine link groups showing longer steps than amine link groups. We model adiabatic junction evolution by discrete steps, with structure determined by energy minimization in a DFT approach and the low bias junction conductance at each step computed using a Green's function approach. We identify different mechanisms whereby the attachment point to the electrode can shift while maintaining similar conductance, explaining why conductance steps can extend over distances of several angstroms. Phosphine and amine link groups sustain different maximum forces, accounting for key differences in junction evolution.

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