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Probing voltage induced bond rupture in a molecular junction[1]

HAIXING LI, Department of Applied Physics and Applied Mathematics, Columbia University, TIMOTHY SU, NATHANIEL KIM, Department of Chemistry, Columbia University, PIERRE DARANCET, Argonne National Laboratory Center for Nanoscale Materials , JAMES LEIGHTON, MICHAEL STEIGERWALD, COLIN NUCKOLLS, Department of Chemistry, Columbia University, LATHA VENKATARAMAN, Department of Applied Physics and Applied Mathematics, Columbia University — We use scanning tunneling microscope break junction to study electric field breakdown at the single molecule level. We investigate breakdown phenomena in atomic chains composed of Si—Si, Si—O, Si—C, Ge—Ge and C—C bonds that are commonly found in the low-κ dielectric material. We see different bond rupture behaviors in a range of molecular backbones, and use the results from a statistically large number of measurements to determine which bond breaks. We find that Si—Si and Ge—Ge bonds rupture above a 1V bias. We also find that the Si—C bond is more robust than Si—O or Si—Si bond at above 1V. Finally, we illustrate how an additional conductance pathway in parallel to the Si—Si bond changes bond rupture behavior under an electric field. We carry out ab initio calculations on these systems and demonstrate that the mechanism for bond rupture under electric field involves "heating" of the molecule through electron-vibrational mode coupling.

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