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Transport properties and stability of molecular break junctions NIKOLAI SERGUEEV, Vanderbilt University, LEONIDAS TSETSERIS, Vanderbilt University, Aristotle University of Thessaloniki, KALMAN VARGA, Vanderbilt University, SOKRATES PANTELIDES, Vanderbilt University, Oak Ridge National Laboratory — The electrode-molecule interface in a break junction is known to be crucial to understand its electronic and transport properties. Using first-principles calculations we first probe a comprehensive set of mechanisms responsible for the stability of the prototype junction of a benzene-dithiol (BDT) between gold electrodes. We find that by pulling the electrodes apart the geometry of the molecule depends drastically on the electrode-surface morphology. We next report results of the quantum transport calculations for several stable junction configurations. The calculations are performed using the recently developed technique based on density functional theory and complex absorbing potentials[1]. The molecular junction is treated as a closed system with a set of complex potentials mimicking the source and the drain electrodes. We find that the conductance of the BDT molecule varies significantly within the different junction configurations. We will compare the results with recent experiments on BDT break junctions. [1]. K. Varga and S.T. Pantelides, PRL 98, 076804 (2007).

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