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Revealing the role of anchoring groups in the electrical conduction through single-molecule junctions ARTUR ERBE, Forschungszentrum Dresden-Rossendorf, LINDA ZOTTI, Universidad Autónoma de Madrid, THOMAS KIRCHNER, University of Konstanz, JUAN-CARLOS CUEVAS, Universidad Autónoma de Madrid, FABIAN PAULY, Universität Karlsruhe, THOMAS HUHN, ELKE SCHEER, University of Konstanz — Using the mechanically controllable breakjunction technique we have performed transport experiments through single ethyne molecules attached to gold electrodes via thiol, nitro, and cyano anchoring groups. We have measured current-voltage characteristics inside a liquid cell. By fitting the experimental curves to a single-level resonant tunneling model we are able to extract both the position of the molecular orbital closest to the Fermi energy and the strength of the metal-molecule coupling. We compare the results to ab initio calculations which give further insight into the transport properties. The dependence of the I-V characteristics on the various anchoring groups shows clearly that these groups affect the coupling strength between metal and the molecules as well as the position of the molecular energy levels.

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