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Modeling of N@C_{60} single-molecule transistors CARSTEN TIMM, University of Kansas, JACOB E. GROSE, Cornell University, WOLFGANG HARNEIT, Free University Berlin, DANIEL C. RALPH, Cornell University — We report on recent experimental and theoretical results for single-molecule transistors involving endohedral N@C_{60} fullerene molecules. In this talk, we will focus on the theoretical modeling. The observed differential conductance shows strong evidence for the exchange interaction between electrons in the fullerene LUMO and the nitrogen p-electrons, favoring an antiferromagnetic interaction. In addition, soft vibrational modes are seen, which are attributed to oscillations of the molecule as a whole. We discuss a model Hamiltonian that reproduces the main features of the experimental conductance.

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