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Single molecular NDR: A first principles study[1] RANJIT PATI, Department of Physics, Michigan Technological University, Houghton, MI 49931 — The demonstration of single molecule switch with a negative differential resistance (NDR) feature has drawn considerable attention in recent years. The NDR feature is described by a steady increase followed by a decrease in current with the increase in applied bias. Here we report a single molecular NDR in a strongly coupled metal-molecule junction, with peak to valley ratio (PVR) of 2.7 at both positive and negative bias. The bias dependent screening effect is explicitly included in our calculation through a rigorous self-consistent many body approach. The non equilibrium Green function approach is used to calculate the quantum transport. The origin of high PVR will be discussed.

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