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**Ab-initio study of transport in the Coulomb-blockade regime** HAITAO WANG, OSAMU HINO, GARNET CHAN, Cornell University — Here we report a new ab-initio model for molecular conductance in the Coulomb blockade regime using unrestricted Hartree-Fock theory within the non-equilibrium Greens function (NEGF) formalism. We demonstrate calculations on recent experimentally studied transition metal complexes, studying the effect of gating on current and the corresponding Coulomb blockade effects.

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