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Effective capacitance of small molecules and nanoscale devices in an electric circuit[1] XIAOGUANG ZHANG, Oak Ridge National Laboratory, JUN-QIANG LU, University of Puerto Rico-Mayaguez, SOKRATES PANTELIDES, Vanderbilt University — A quantum-mechanical definition of the capacitance of a molecule or nanodevice between two electodes is complicated by the fact that one cannot unambiguously partition the electron density between the metal electrodes and the molecule or device. We introduce a procedure that leads to an unambiguous partitioning and to practical calculations using a linear response formalism for alternating current (AC) transport. The linear response theory is derived for a closed quantum system including the molecule and two electrodes with a finite length. The mutual capacitance between the two electrodes in the absence of a molecule or device is subtracted to obtain an effective capacitance for the molecule in the presence of the electrodes. Numerical calculations show that the effective capacitance converges with the increasing length of the electrodes. The converged results for single molecules of CO_2, CO, CH_4, NH_3, H_2, H_2O, and benzene range from 0.18 to 2.832 (10^{-22} F).

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