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Constrained LDA ab-initio calculation of screening of charging energy in C60 JAY SAU, JEFFREY NEATON, K.H. KHOO, Department of Physics UC Berkeley, HYOUNG CHOI, Department of Physics, Yonsei University, STEVEN LOUIE, MARVIN COHEN, Department of Physics UC Berkeley — Recent measurements and theoretical calculations of the electronic properties of C60 on metal substrates have shown that the electron-electron repulsion parameter U, which determines the coulomb blockade transport properties, is strongly screened in the presence of a metal susbtrate. Since standard Density Functional Theory calculations treat this charging energy in a mean field sense, it ignores the discreteness of the charge on the C60 that is critical to coulomb blockade. To account for the effect of the screened U in transport experiments we calculate the charging energy of C60 in a few environments using a constrained LDA approach and explore the implications for coulomb blockade transport phenomena. This work was supported by National Science Foundation Grant No. DMR04-39768 and by the Director, Office of Science, Office of Basic Energy Sciences, Division of Material Sciences and Engineering, U. S Department of Energy under Contract No. DE-AC03-76SF00098. Computational resources have been provided by DOE at the National Energy Research Scientific Computing Center(NERSC)

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