Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Substrate Screening Effects in *ab initio* Many-body Green's Function Calculations of Doped Graphene on SiC[1] DEREK VIGIL-FOWLER, JOHANNES LISCHNER, STEVEN LOUIE, University of California, Berkeley and Lawrence Berkeley National Lab — Understanding many-electron interaction effects and the influence of the substrate in graphene-on-substrate systems is of great theoretical and practical interest. Thus far, both model Hamiltonian and ab initio GW calculations for the quasiparticle properties of such systems have employed crude models for the effect of the substrate, often approximating the complicated substrate dielectric matrix by a single constant. We develop a method in which the spatially-dependent dielectric matrix of the substrate (e.g., SiC) is incorporated into that of doped graphene to obtain an accurate total dielectric matrix. We present ab initio GW + cumulant expansion calculations, showing that both the cumulant expansion (to include higher-order electron correlations) and a proper account of the substrate screening are needed to achieve agreement with features seen in ARPES. We discuss how this methodology could be used in other systems.

[1]This work was supported by NSF Grant No. DMR10-1006184 and U.S. DOE Contract No. DE-AC02-05CH11231. Computational resources have been provided by the NERSC and NICS. D.V-F. acknowledges funding from the DOD's NDSEG fellowship.

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Date submitted: 08 Nov 2012 Electronic form version 1.4