Long-range Coulomb interactions in surface systems: a first principles description within self-consistently combined GW and dynamical mean field theory

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Systems of adatoms on semiconductor surfaces display competing ground states and exotic spectral properties typical of two-dimensional correlated electron materials which are dominated by a complex interplay of spin and charge degrees of freedom. We report a fully ab initio derivation of low energy Hamiltonians for the adatom systems Si(111):X, with X=Sn, Si, C, Pb, that we solve within self-consistent combined GW and dynamical mean field theory ("GW+DMFT") [1]. Calculated photoemission spectra are in agreement with available experimental data. We rationalize experimentally observed tendencies from Mott physics towards charge-ordering along the series as resulting from substantial long-range interactions.

[1] P. Hansmann, T. Ayral, L. Vaugier, P. Werner, and S. Biermann, arXiv:1301.4325 (to be published in PRL)