Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Real-space methods for calculating the electronic response of 2D materials[1] BENJAMIN GARRETT, JAMES CHELIKOWSKY, University of Texas at Austin — We study the effects of applied fields on several 2D materials including graphene and metal dichalcogenides. We use a real space density functional method with 2D periodic boundary conditions. This negates the need for a supercell and allows us to directly simulate a transverse electric field. The dielectric properties can be calculated without layer-layer interactions. Changes in band structure in response to imposed fields are also discussed.

[1]This work is supported by DOE grant DE-FG02-06ER46286. Computational resources were provided by NERSC.

James Chelikowsky
Univ of Texas, Austin

Date submitted: 13 Nov 2014 Electronic form version 1.4