Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Exciton and trions binding energies in single-layer MoS_2: applications of the density-matrix time dependent density[1] ALFREDO RAMÍREZ-TORRES, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics, University of Central Florida, Orlando, Florida 32816, USA — Exciton and trion binding energies of a single layer of MoS_2 are studied using a time- dependent density-functional theory formalism. Kohn-Sham orbitals of the initial state were obtained using ab initio electronic structure calculations based on density functional theory. Several types of exchange-correlation (XC) kernels are implemented in our code to compare their performance. As expected our results depend crucially on the XC kernels used. In particular, the exchange-only adiabatic local density approximation kernel results in the binding energy about 0.1 eV, which is smaller than those obtained using the GW theory approximation ($\sim$ 0.9 eV) [1]. We have generalized the approach on the case of trion excitations, which gives the trion binding energy $\sim$ 0.3eV when one used the LDA approximation. On the other hand, we demonstrate that the results for the experimental binding energies can be reproduced by using phenomenological local and long-range XC kernels. [1] T. Cheiwchanchamnangij and W. R. L. Lambrecht, Phys. Rev. B **85**, 205302 (2012).

[1]This work was partially supported by CONACYT México (184722) and DOE grant DE-FG02-07ER46354

Duy Le
Department of Physics, University of Central Florida,
Orlando, Florida 32816, USA

Date submitted: 03 Jan 2013 Electronic form version 1.4