Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Role of weak interactions in phase transitions of layered transition metal dichalcogenides: An ab initio study NILADRI SENGUPTA, ADRIENN RUZSINSZKY, JOHN P. PERDEW, Temple Univ — Phase transitions of layered materials are not often clearly explained and captured by the GGA level density functional calculations. Weak interactions might play an important role in these phase transitions. Now GGA can not describe well weak interactions. So we intend to use several new meta GGAs (TPSS, RevTPSS, MS family etc.), many body VDW corrected meta GGAs and RPA to study phase transitions of layered transition metal dichalcogenides (ME_2 ; M = Ti, V, Cr, Ta, Mo, W ; E = Se, S, Te) and investigate the role of weak interactions in those cases.

Niladri Sengupta
Temple Univ

Date submitted: 14 Nov 2014 Electronic form version 1.4