Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Stability of two-dimensional BN-Si structures ERNESTO SANDOVAL, SAMAD HAJINAZAR, ALEKSEY KOLMOGOROV, State Univ of NY - Binghamton — We have used *ab initio* modeling to examine stability factors in two-dimensional (2D) CSi, BNC_2, and recently proposed $BNSi_2$ honeycomb structures. We have found that the lack of miscibility in the last two systems is due to limited involvement of nitrogen electronic states in the covalent bonding. Our evolutionary ground state searches uncovered that in the $(BN)_xSi_{1-x}$ pseudobinary system non-honeycomb flat structures have lower energy than the graphene-like configurations. Nevertheless, none of these or previously proposed polymorphs have been found to be stable with respect to phase separation into 2D Si and BN.

Ernesto Sandoval
State Univ of NY - Binghamton

Date submitted: 11 Nov 2016 Electronic form version 1.4