Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Structural and Electronic Properties of BC 3 with Van der Waals Density Functional Theory[1] BURAK OZDEMIR, VERONICA BARONE, Central Michigan Univ — Layered materials have attracted a lot of attention recently due to their unique properties that can be optimized for technological applications such as energy storage and transparent conductors. Among these materials, a graphite-like BC3 (g-BC3) structure has been recently under investigation as it provides a similar morphology than graphite but with a large concentration of electron deficient B atoms. Despite the recent experimental and theoretical works, the morphology of this materials is still not well undertsood. In this work, stable stacking configurations of g-BC3 have been determined using different exchange-correlation functionals that include dispersion corrections. We identify the most stable structures and characterize their electronic properties.

[1]We acknowledge the support from NSF-CBET-1335944

Burak Ozdemir
Central Michigan Univ

Date submitted: 13 Nov 2014 Electronic form version 1.4