Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Size dependence in the stabilities and electronic properties of graphyne and its BN analogue V. ONGUN OZCELIK, SALIM CIRACI, Bilkent Univ — We predict the stabilities of α-graphynes and their boron nitride analogues(α-BNyne), which are considered as competitors of graphene and two-dimensional hexagonal BN [1]. Based on first-principles plane wave method, we investigated the stability and structural transformations of these materials at different sizes using phonon dispersion calculations and ab-initio finite temperature, molecular dynamics simulations. Depending on the number of additional atoms in the edges between the corner atoms of the hexagons, n, both α-graphyne(n) and α-BNyne(n) are stable for even n, but unstable for odd n. α-graphyne(3) undergoes a structural transformation, where the symmetry of hexagons is broken. We present the structure optimized cohesive energies, electronic, magnetic and mechanical properties of stable structures. Our calculations reveal the existence of Dirac cones in the electronic structures of α-graphynes of all sizes, where the Fermi velocities decrease with increasing n. The electronic and magnetic properties of these structures are modified by hydrogenation.

[1] V. Ongun Ozcelik and S. Ciraci, J. Phys. Chem. C, 2013, 117 (5), pp 2175-2182.

V. Ongun Ozcelik
Bilkent Univ

Date submitted: 15 Nov 2013 Electronic form version 1.4