Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Self-assembly mechanisms and even/odd disparity of short atomic chains on graphene[1] V. ONGUN OZCELIK, SALIM CIRACI, Bilkent University — Self-assembly mechanisms of carbon chains on boron nitride and short BN chains on graphene are investigated using first-principles plane wave calculations. Once a C_2 nucleates on h-BN, the insertion of each additional carbon at its close proximity causes a short segment of carbon atomic chain to grow by one atom at a time in a quaint way: The existing chain leaves its initial position and subsequently is attached from its bottom end to the top of the carbon ad-atom. The electronic, magnetic and structural properties of these chains depend on the number of carbon atoms in the chain, such that they exhibit an even-odd disparity. An individual carbon chain can also modify the electronic structure with localized states in the wide band gap of h-BN. As a reverse situation, the growth of short BN atomic chains on graphene is also examined. These results reveal the interesting self-assembly behavior short atomic chains. Furthermore, we find that these atomic chains enhance the chemical activity of h-BN and graphene sheets by creating active sites and can act as pillars between two and multiple sheets of these honeycomb structures leaving wider spacing between them to achieve high capacity storage of specific molecules.

[1] V.O. Ozcelik and S. Ciraci, Phys. Rev. B 86 155421 (2012).

[1]This research was supported by the Academy of Sciences of Turkey(TUBA) and the Scientific and Technological Research Council of Turkey(TUBITAK).

V. Ongun Ozcelik
Bilkent University

Date submitted: 08 Nov 2012 Electronic form version 1.4