Abstract Submitted
for the 4CF11 Meeting of
The American Physical Society

Strain-modulated Fermi velocity of charge carriers in 2D graphene: A first principles study KASON ASHE, XIHONG PENG, Arizona State University — Using first principles density-functional theory calculations, we have shown that the Fermi velocity of charge carriers in two-dimensional graphene is tunable. Three different types of strain were studied. They are uniform biaxial strain, uniaxial strain in the armchair direction, and uniaxial strain in the zig-zag direction. We found by applying strains, particularly uniform biaxial type, the Fermi velocity can be modified by an appreciable amount. The Fermi velocity increases when biaxial compression is applied. For example, the Fermi velocity increases 33% under 12% compression. Conversely, the Fermi velocity was shown to decrease by as much as 19% when the graphene was expanded uniformly by up to 12%. In the case of uniaxial strain in the zig-zag direction, it is shown the Dirac point is no longer located at K but near R from the band structure and with a greater amount of strain the Dirac point moves further away from R toward S. As graphene is stretched in the armchair direction the Dirac point moves away from K towards Γ. These results suggest an effective way to tune the Fermi velocity of graphene.

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Date submitted: 15 Sep 2011 Electronic form version 1.4