Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Ferromagnetically coupled local moments along an extended line defect in graphene[1] CARTER T. WHITE, NRL, SMITHA VASUDEVAN, GWU, DANIEL GUNLYCKE, NRL — Recently an extended line defect was observed composed of octagonal and pentagonal carbon rings embedded in a graphene sheet [Nat. Nanotech. 5, 326 (2010)]. We report results of studies we have made of this defect using both first-principles and semi-empirical methods. Two types of boundary-localized states arising from the defect are identified. The first (second) type has eigenstates with wavefunctions that are anti- symmetric (symmetric) with respect to a mirror plane that is perpendicular to the graphene sheet and passes through the line defect center line. The boundary-localized anti-symmetric states are shown to be intimately connected to the zigzag edge states of semi-infinite graphene. They exhibit little dispersion along the defect line and lie close to the Fermi level giving rise to a spontaneous spin polarization along the defect once electron-electron interactions are included at the level of a mean field approximation to a Hubbard Model. Within this approach, symmetry requires that the principal moments couple ferromagnetically both along and across the line defect leading to approximately 2/3 more up than down spin electrons per defect repeat unit.

[1]This work was supported by ONR, directly and through NRL.

Carter T. White
NRL

Date submitted: 19 Nov 2010 Electronic form version 1.4