

Abstract Submitted  
for the MAR10 Meeting of  
The American Physical Society

**Magnetism of nitrogen-vacancy complexes in epitaxial graphene on SiC(0001)**<sup>1</sup> S. H. RHIM, Y. QI, G. F. SUN, Y. LIU, M. WEINERT, L. LI, U. Wisconsin-Milwaukee — We present a study of the magnetism of nitrogen impurity–vacancy complexes in epitaxial graphene on SiC(0001) using a combination of density functional calculations and scanning tunneling microscopy. Nitrogen-vacancy complexes are created by means of a nitrogen plasma. From the calculated energetics and by comparison with STM, the most probable configuration is found to have the vacancy and substitutional nitrogen at the nearest neighbor site. This configuration is non-magnetic, whereas other higher energy N-vacancy configurations (and the isolated vacancy) are magnetic. Adatoms such as H, C, and N, in combination with the nitrogen-vacancy complex, show a variety of magnetic behaviors, depending on both the adatom and its position.

<sup>1</sup>Supported by DOE (DE-FG02-05ER46228) and NSF (DMR-0706359)

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Date submitted: 19 Nov 2009

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