

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

The role of vacancies in Li-intercalated bilayer graphene¹ R. EMMETT KAHN², Physics Department, Reed College, ANDREW O'HARA, YUYANG ZHANG, SOKRATES T. PANTELIDES, Department of Physics and Astronomy, Vanderbilt University — Recently, there has been increased interest in graphene for device applications both on its own and stacked with other 2D materials. Doping graphene via adsorption of lithium can shift the Fermi energy in graphene, effectively changing it from a semimetal to a metal. As an alternative to adsorption and to prevent contamination of the rest of the device stack, lithium can be intercalated between two layers of graphene. In this work, we investigate, using density functional theory, the possibility for lithium to migrate through defects in the graphene lattice and the role that excess layers play on the migration barriers. We found that there is a significant increase in the energy barrier for the pass-through of lithium of 0.26 eV when lithium leaves a bilayer through a divacancy vs when it passes through a divacancy in a monolayer, suggesting that the presence of the second layer minimizes defect migration. Furthermore, the presence of asymmetry in the energy barrier for certain defect types suggests the possibility of using defects to fabricate thermally intercalated bilayers.

¹Supported by NSF Grant DMR-1508433

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Date submitted: 11 Nov 2016

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