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Altering graphene line defect properties using chemistry[1] SMITHA VASUDEVAN, George Washington University, CARTER WHITE, DANIEL GUNLYCKE, Naval Research Laboratory — First-principles calculations are presented of a fundamental topological line defect in graphene that was observed and reported in Nature Nanotech. 5, 326 (2010). These calculations show that atoms and smaller molecules can bind covalently to the surface in the vicinity of the graphene line defect. It is also shown that the chemistry at the line defect has a strong effect on its electronic and magnetic properties, e.g. the ferromagnetically aligned moments along the line defect can be quenched by some adsorbates. The strong effect of the adsorbates on the line defect properties can be understood by examining how these adsorbates affect the boundary-localized states in the vicinity of the Fermi level. We also expect that the line defect chemistry will significantly affect the scattering properties of incident low-energy particles approaching it from graphene.

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