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Graphene symmetry-breaking with molecular adsorbates: modeling and experiment[1] M.A. GROCE, M.K. HAWKINS, Y.L. WANG, W.G. CULLEN, T.L. EINSTEIN, U. of Maryland — Graphene's structure and electronic properties provide a framework for understanding molecule-substrate interactions and developing techniques for band gap engineering. Controlled deposition of molecular adsorbates can create superlattices which break the degeneracy of graphene's two-atom unit cell, opening a band gap. We simulate scanning tunneling microscopy and spectroscopy measurements for a variety of organic molecule/graphene systems, including pyridine, trimesic acid, and isonicotinic acid, based on density functional theory calculations using VASP. We also compare our simulations to ultra-high vacuum STM and STS results.

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