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A theoretical study of symmetry-breaking organic overlayers on single- and bi-layer graphene[1] JOSUE MORALES-CIFUENTES, T.L. EINSTEIN, Physics & CMTC, Univ. Maryland, College Park — An "overlayer" of molecules that breaks the AB symmetry of graphene can produce (modify) a band gap in single- (bi-) layer graphene.[2] Since the triangular shaped trimesic acid (TMA) molecule forms two familiar symmetry breaking configurations, we are motivated to model TMA physisorption on graphene surfaces in conjunction with experiments by Groce et al. at UMD. Using VASP, with ab initio van der Waals density functionals (vdW-DF), we simulate adsorption of TMA onto a graphene surface in several symmetry-breaking arrangements in order to predict/understand the effect of TMA adsorption on experimental observables.

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[2]M. Li et al., Phys. Rev. B 76, 155438 (2007)

Josue Morales-Cifuentes
Physics & CMTC, Univ. Maryland, College Park

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