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Optical properties of functionalized monolayer and bilayer graphene JINLUO CHENG, CUAUHTÉMOC SALAZAR, JOHN E. SIPE, Department of Physics and Institute for Optical Sciences, University of Toronto, 60 St. George Street, Toronto, Ontario, Canada M5S 1A7 — We use *ab initio* calculations to investigate the structures, band structures, and optical properties of functionalized monolayer and bilayer graphene, where a hydrogen atom is attached to only one carbon atom site periodically every few unit cells. The hydrogen atom distorts the carbon atoms vertically, but the inplane structure is approximately unchanged. The ground state acquires a bandgap due to adsorption depending on the supercell size, and shows magnetic order, which is in agreement with a recent experiment [1]. The calculated optical absorption spectra displays detailed structures at lower photon frequencies than that of the pristine graphene.

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