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The Electronic Structure on Two-Dimensional Graphane from Ab Initio Theory JIN ZHAO, HRVOJE PETEK — Using density functional theory (DFT) we have investigated the electronic structure of the intrinsic two-dimensional graphane and fluorine-substituted graphane. We found the conduction band minimum of graphane has nearly free electron (NFE) properties similar, but in some respects different, than the recently calculated image potential states of graphene and superatom states of fullerenes.[1,2] The electronic structure of fluorine-substituted graphane is very sensitive to the doping configuration. The band gap of fluorine doped graphane can be tuned by different doping functionalization. Our study gives new insights into engineering of the electronic structure of two-dimensional semiconductors by surface chemical functionalizaton.

[1]V. M. Silkin, J. Zhao, F. Guinea, E. V. Chulkov, P. M. Echenique, and H. Petek, Phys. Rev. B **80**, 121408 (2009)
[2]M. Feng, J. Zhao, and H. Petek, Science **320**, 359 (2008)

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