Abstract Submitted
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Few-layer and symmetry-breaking effects on the electrical properties of ordered CF_3Cl phases on graphene[1] JOSUE MORALES-CIFUENTES, Physics & CMTC, UMCP, YILIN WANG, Physics, UMCP, JANICE REUTT-ROBEY, Chemistry & Biochemistry, UMCP, T.L. EINSTEIN, Physics & CMTC, UMCP — An effective pseudopotential mechanism for breaking the inherent sublattice symmetry of graphene has been studied using DFT calculations on hexagonal boron nitride.[2] Electrical detection of CF_3Cl phase transitions on graphene shows the existence of a commensurate ordered phase in which this can be tested.[3] We study the electronic properties of this phase using VASP ver 5.3.3, with ab initio van der Waals density functionals (vdW-DF1 and vdW-DF2).[4] [5]Consistent with a physisorbed phase, binding energies and charge transfer per CF_3Cl molecule are calculated to be on the order of 280meV and 0.01e, respectively. By exploring different coverages and orientations of this ordered phase we are able to open a band gap in some configurations; said gap is in the range of 8 to 80meV depending on the strength of the effective pseudopotential. Furthermore, we calculate the screening of these effects in bi-layer and tri-layer graphene.

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[2]Gianluca Giovannetti et al. , PRB 76, 073103 (2007)
[3]Yilin Wang et al. , APL 103, 201606 (2013)
[4]Jiří Klimeš et al. , PRB 83, 195131 (2011)
[5]Kyuho Lee et al. , PRB 82, 081101(R) (2010)

Josue Morales Cifuentes
Univ of Maryland-College Park

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