Abstract Submitted
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First-Principle Calculations of The Conductivity of Br-Doped Graphite[1] RASHID HAMDAN, CHAO CAO, ALEXANDER KEMPER, HAI-PING CHENG — First-principles calculations are used to study the enhanced in-plane conductivity that was observed experimentally in Br-doped graphite systems.[2] The band structure near the Fermi surface of the doped systems with different bromine concentrations compared to that of pure graphite, and the charge transfer between carbon and bromine atoms are analyzed to understand the conductivity change in the different directions. In addition, we address the effect of the compression of graphite layers on the stability of the bromine molecule Br_2 between these layers and thus on the conductivity of the system. Our calculations show that for large separation between doped graphite layers bromine is more stable in the molecular form (Br_2) and has a negligible effect on in- plane conductivity. However, with increased compression (decreased layer-layer separations) Br_2 molecule tend to dissociate and exchange charge with the nearby graphite layers causing an increase in hole conductivity.

[1]US/DOE/BES/DE-FG02-02ER45995, computational centers: UF-HPC/ NERSC.
[2]Tongay et al. Phys. Rev. B 81, 115428 (2010)

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