

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Reactivity of Graphene Investigated by Density-Functional Theory¹ HIMADRI SONI, JULIAN GEBHARDT, ANDREAS GRILING, Friedrich-Alexander Universitt Erlangen-Nrnberg, CHAIR OF THEORETICAL CHEMISTRY TEAM — Using spin-polarized density-functional theory, we study the adsorption and reaction of hydrogen and fluorine with graphene. Graphene has a bipartite lattice with two different sublattices and hence, due to Lieb's theorem, the inequality between two sublattices should lead to a net magnetic moment upon adsorption of hydrogen or fluorine. Our calculations using density-functional theory with the generalized gradient approximation predict a magnetic moment of 1 B for a single hydrogen adsorbed on graphene but not for a single fluorine atom adsorbed on graphene. Switching to hybrid density-functional theory with the HSE functional [1], we obtain a magnetic moment of 1 B for a single fluorine atom adsorption on graphene. This is in line with work of Kim et al. [2], who also found in density-functional theory calculations with the HSE exchange-correlation functional spin-polarization for a fluorine adatom on graphene. Here, we present a systematic study of the reactivity and relevant adsorption mechanism for single-sided graphene, i.e., a graphene sheet which is accessible by an adsorbate from only one side with hydrogen and fluorine using hybrid density-functional theory. References 1)AV Krukau et al., J. Chem. Phys. 125,224106(2006) 2)H-J Kim et al., Phys. Rev B 87,174435(2013)

¹German Research Council (DFG) by the Collaborative Research Center 953

Himadri Soni
Friedrich-Alexander Universitt Erlangen-Nrnberg

Date submitted: 05 Nov 2015

Electronic form version 1.4