

# On the Electronic and Optical Properties of Fluorographene, Chlorographene, and Graphane

Frantisek Karlicky, Michal Otyepka

<sup>1</sup>Regional Centre of Advanced Technologies and Materials, Department of Physical Chemistry, Faculty of Science, Palacky University, 17. listopadu 12, 771 46 Olomouc, Czech Republic  
[frantisek.karlicky@upol.cz](mailto:frantisek.karlicky@upol.cz)

## Abstract

New two-dimensional materials derived from graphene by attachment of hydrogen and halogens have attracted considerable interest over the past few years because of their potential applications (e.g., in electronic devices). [1] Here, we consider presence of point defects and the effect of electron-electron and electron-hole correlation on the electronic/optical properties of materials under study. Especially, large difference between the experimental optical gap and the electronic band gap from many-body GW theory for fluorographene [2,3] was explained by unusual large binding energies of excitons, whereas point defects lowered band gaps and absorption energies only slightly. [4] Similar effects are predicted for chlorographene, which stability is, however, still questionable. [5]

## References

- [1] Karlicky F., Datta KKR., Otyepka M., Zboril R., ACS Nano **7** (2013) 6434
- [2] Nair RR., Ren WC., Jalil R., Riaz I., Kravets VG., Britnell L., Blake P., Schedin F., Mayorov AS., Yuan SJ., Katsnelson MI., Cheng HM., Strupinski W., Bulusheva LG., Okotrub AV., Grigorieva IV., Grigorenko AN., Novoselov KS., Geim AK., Small **6** (2010) 2877
- [3] Zboril R., Karlicky F., Bourlinos AB., Steriotis TA., Stubos AK., Georgakilas V., Safarova K., Jancik D., Trapalis C., Otyepka M., Small **6** (2010) 2885
- [4] Karlicky F., Otyepka M., J. Chem. Theory Comput. **9** (2013) 4155
- [5] Karlicky F., Zboril R., Otyepka M., J. Chem. Phys. **137** (2012) 034709

## Figure

