Graphene halides: properties and applications

Frantisek Karlicky,[1] Athanasios B. Bourlinos,[1,2] Michal Otyepka[1] and Radek Zboril[1]

[1]Regional Centre of Advanced Technologies and Materials, Department of Physical Chemistry, Faculty of Science, Palacky University, 17. listopadu 12, 771 46 Olomouc, Czech Republic
[2]Institute of Materials Science, NCSR "Demokritos", g. Paraskevi Attikis, 15310 Athens, Greece
frantisek.karlicky@upol.cz

Abstract

Graphene, a single-layer carbon sheet, has been regarded as one of the most promising candidates for next generation electronic materials due to its extremely high mobility of electrical carrier. However, graphene lacks a band-gap around Fermi level, which is defining concept for semiconductor materials and essential for controlling the conductivity by electronic means [1]. One of the ways to band-gap opening, i.e. covalently modified graphene derivatives prepared by attachment of hydrogen, halogens or other atoms have been of broad interest for their potential applications (e.g. in electronic devices) in the last few years [2]. The relative simplicity of atomic adsorbates allows them to be also well described by theoretical calculations.

Here we review recent progress on graphene halides field and focus on structural and vibrational properties [3-5], which are simultaneously fingerprints of considered materials, whereas electronic, optical, thermodynamical and mechanical properties [5-8] of graphene halides are important from application perspective. E.g. the zero band gap of graphene is opened by hydrogenation and halogenation and strongly depends on the chemical composition of mixed graphene halides. The stability of graphene halides decreases sharply with increasing size of the halogen atom [7,8]. Periodic hybrid DFT calculations on graphane and stoichiometrically halogenated graphene derivatives predict that fluorographene is most stable 2D insulator, whereas graphene iodide spontaneously decomposes in agreement with results obtained in our experimental laboratories [3,4]. In terms of band gap and stability, promising materials are suggested, e.g., for (opto)electronics applications, because band gaps of such derivatives are similar to those of conventional semiconductors, and they are expected to be stable under ambient conditions (Figure 1).

References

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Figures

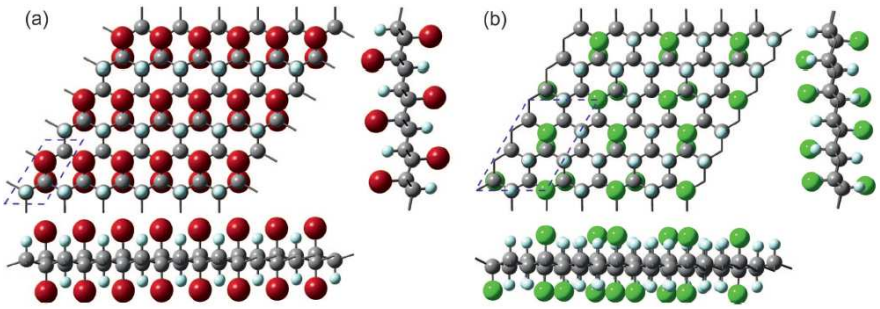

Figure 1: Schematic view of selected promising compounds whose stability is expected (carbon, fluorine, chlorine, and bromine atoms are shown as black, blue, green, and red spheres, respectively).