Electronic properties of fluorinated graphite and graphene

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Depending on synthesis method graphite fluorides CF_x (x ≤ 1) with different composition can be obtained. In the stoichiometric compounds, CF and C₂F, fluorine atoms form covalent bonds with each carbon atom or with half of carbon atoms of a graphene layer. The large interlayer spacing (more than 0.6 nm) allows preparing intercalates with various molecules. Depending on synthesis method graphite fluorides CF_x (x ≤ 1) with different composition can be obtained. The large interlayer spacing (more than 0.6 nm) allows preparing intercalates with various molecules.

Graphite fluoride with a composition close to C₂F has been synthesized by fluorination of highly oriented pyrolytic and natural graphite using a BrF₃ at room temperature. Electronic structure of graphite fluoride was probed using near edge x-ray absorption fine structure (NEXAFS) spectroscopy. The spectra measured near the C K- and F K-edges showed retention of delocalized π^* -system in graphite fluoride C₂F. The probable distribution of fluorine atoms on the graphite surface was determined from quantum-chemical modeling of the NEXAFS spectra. The fluorine atoms were found to be easy detached from the C₂F surface under electron beam irradiation in a high vacuum or with a hydrazine vapor treatment. Resulting restoration of graphene π -system produces channels for electron transport. Surface electric conductivity of C₂F sample was found to appear after ~ 1 min exposure to hydrazine vapor and increase after additional ~40 sec treatment. The dependence of sample resistance on the exposure time is fitted by a triple exponential function exhibiting complex character of the reduction process. Investigation of sensor properties of the reduced C₂F surface to NH₃, NO₂, and Cl₂ was carried out by home-made gas sensing detection system at room temperature. Calculations revealed that NH₃ or NO₂ molecule is readily adsorbed on the reduced surface with a charge transfer from the molecule to the carbon layer or verse versa.

The changes in C_2F_x stoichiometry are shown to have a decisive effect on magnetic properties of produced complexes. The spin concentration decreases with the increase of fluorine content in fluorocarbon matrix. All samples have groups of correlated spins; at the temperatures 1.75–5 K nonlinear magnetization is observed, indicating a high-spin state. Application of the Langevin formula shows that the clusters consiSt of 10–20 interacting spins.