Computational and Impedimetric Studies on Sub-picomolar Ammonia Sensing Using Fluorographene

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Abstract

Single molecule detection using graphene can be brought by tuning the interactions via specific dopants. Electrostatic interaction between the most electronegative element fluorine (F) and hydrogen (H) is one of the strong interactions in hydrogen bonding, and here we report the selective binding of ammonia/ammonium with F in fluorographene (FG) resulting to a change in the impedance of the system. Very low limit of detection value of ~ 0.44 pM with linearity over wide range of concentrations (1 pM – 0.1μM) is achieved using the FG based impedance sensor, and this screen printed FG sensor works in both ionized (ammonium) and un-ionized ammonia sensing platforms. The interaction energies of FG and NH3/NH4+ are evaluated using density functional theory calculations and the interactions are mapped. Here FGs with two different amounts of fluorine contents - ~ 5 atomic% ($C_{39}H_{16}F_2$) and ~ 24 atomic% ($C_{39}H_{16}F_{12}$) - are theoretically and experimentally studied for selective, high sensitive and ultra-low level detection of ammonia. Fast responding, high sensitive, large area patternable FG based sensor platform demonstrated here can open new avenues for the development of point-of-care devices and clinical sensors.

References

[1] Palmqvist, E.; Berggren Kriz, C.; Svanberg, K.; Khayyami, M.; Kriz, K.; Svanberg, M.; K.; Khayyami, M.; Krix, D. Biosens. Bioelectron **10** (1995) 283.

[2] Feher, M.; Martin, P. A.; Rohrbacher, A.; Soliva, A. M.; Maier, J. P. Appl. Opt. **32** (1993) 2028

[3] Ohira, S-I, Toda, K.; Ikebe, S-I, Dasgupta, P. K. Anal. Chem. **74** (20025890