Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Activated carbon-based gas sensors: Effects of surface features on sensing mechanism

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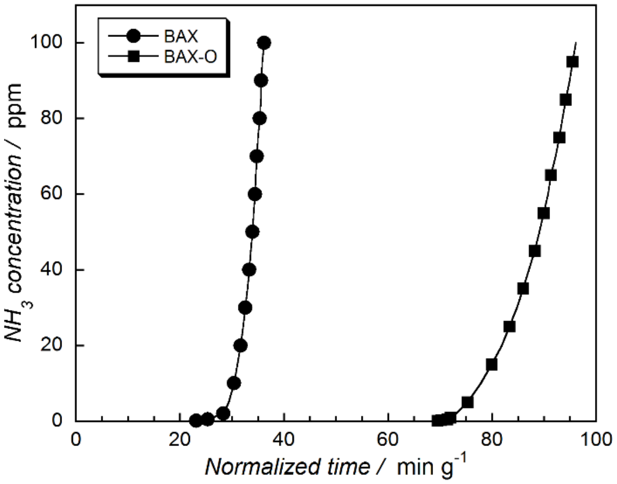

Fig. S1. Ammonia breakthrough curves for BAX and BAX-O carbons.

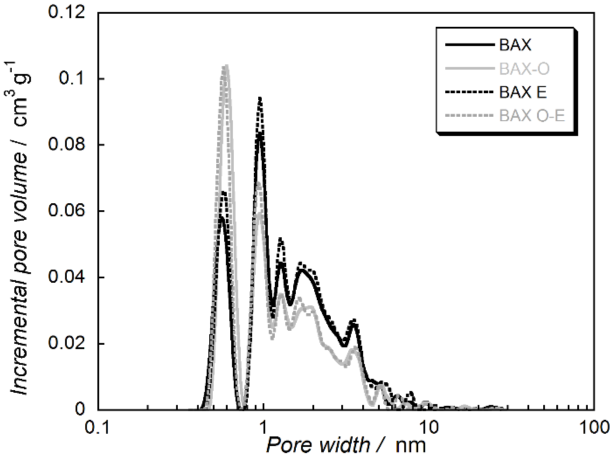

Fig. S2. Pore size distributions for the carbons studied.

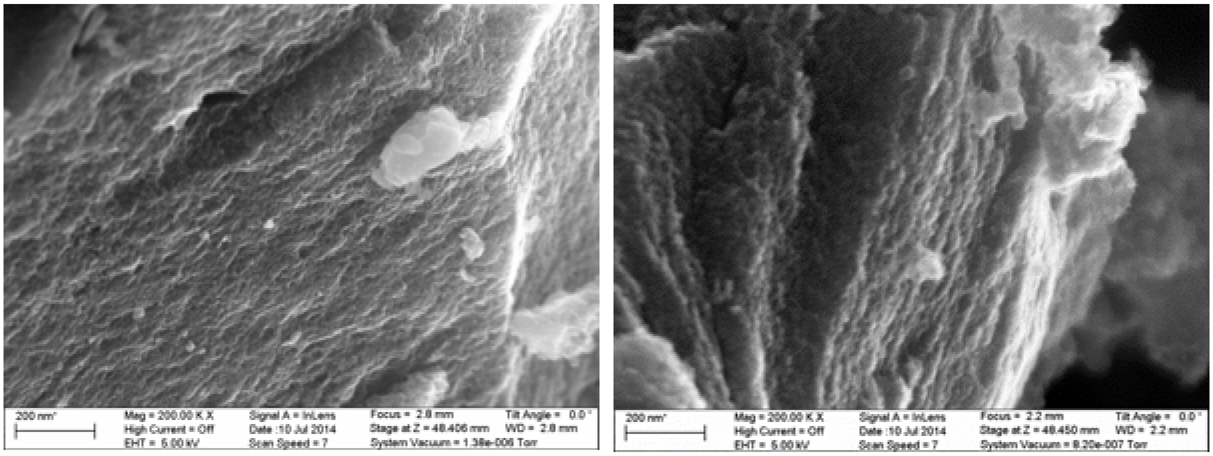

Fig. S3. SEM images of BAX (A) and BAX-O (B).

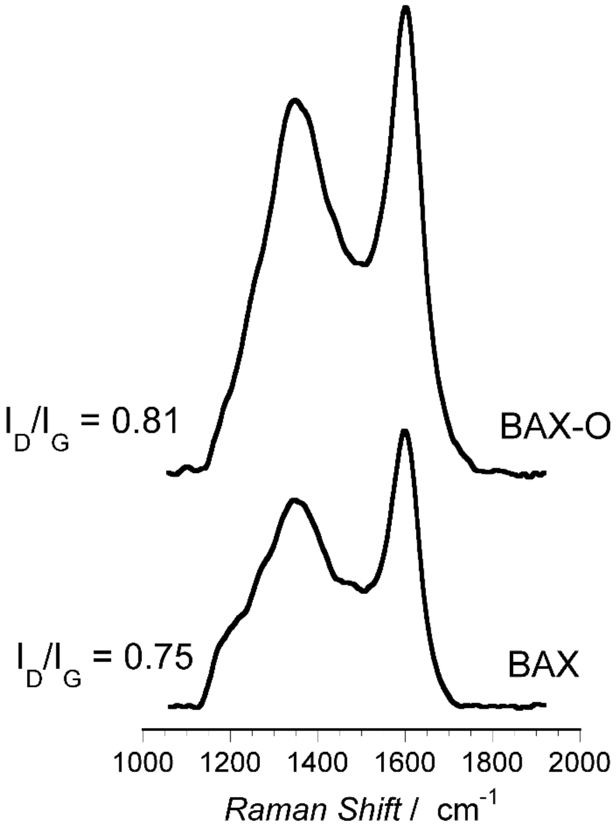

Fig. S4. Raman spectra for BAX and BAX-O.

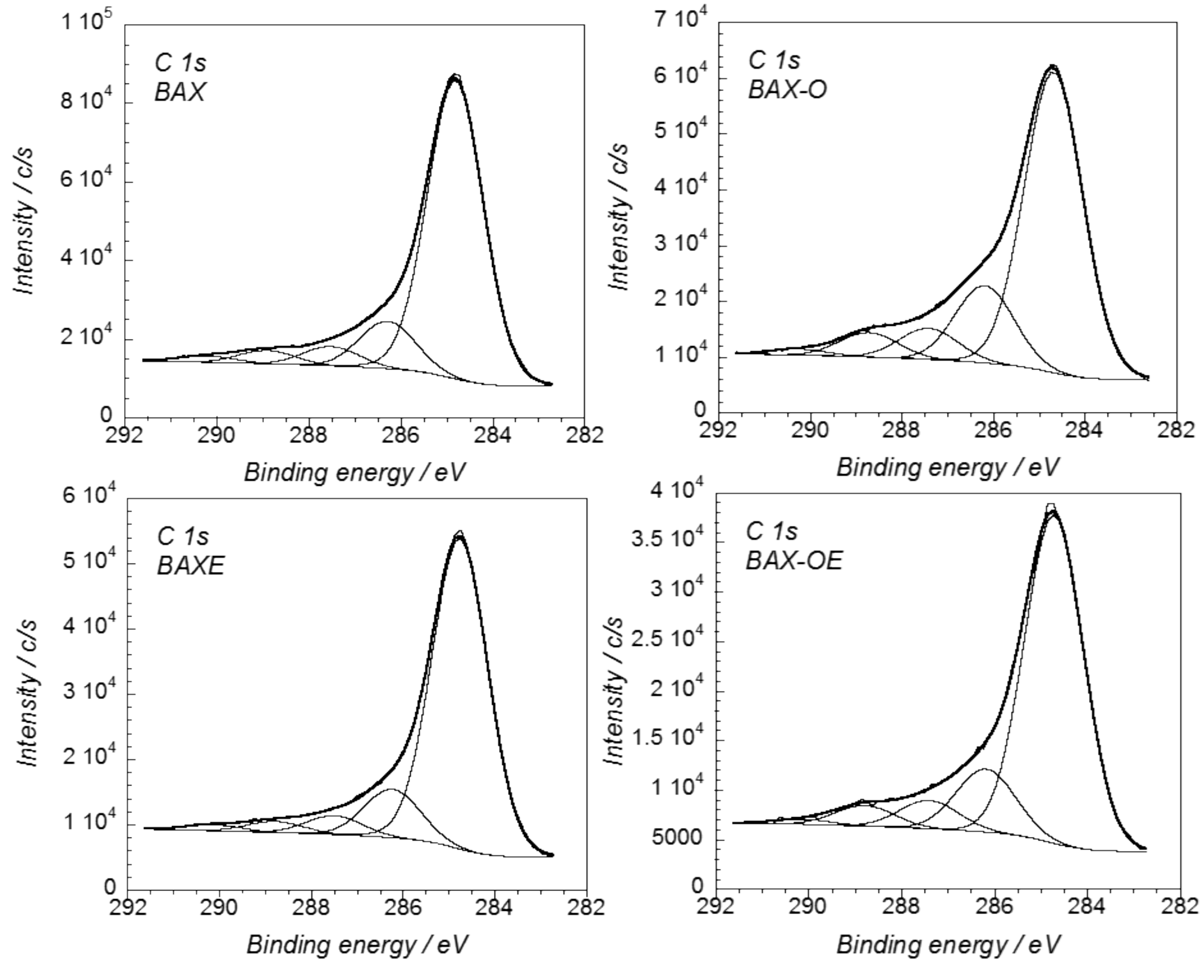

Fig. S5. The deconvolution of C 1*s* core energy levels for the initial and exposed to ammonia carbons.

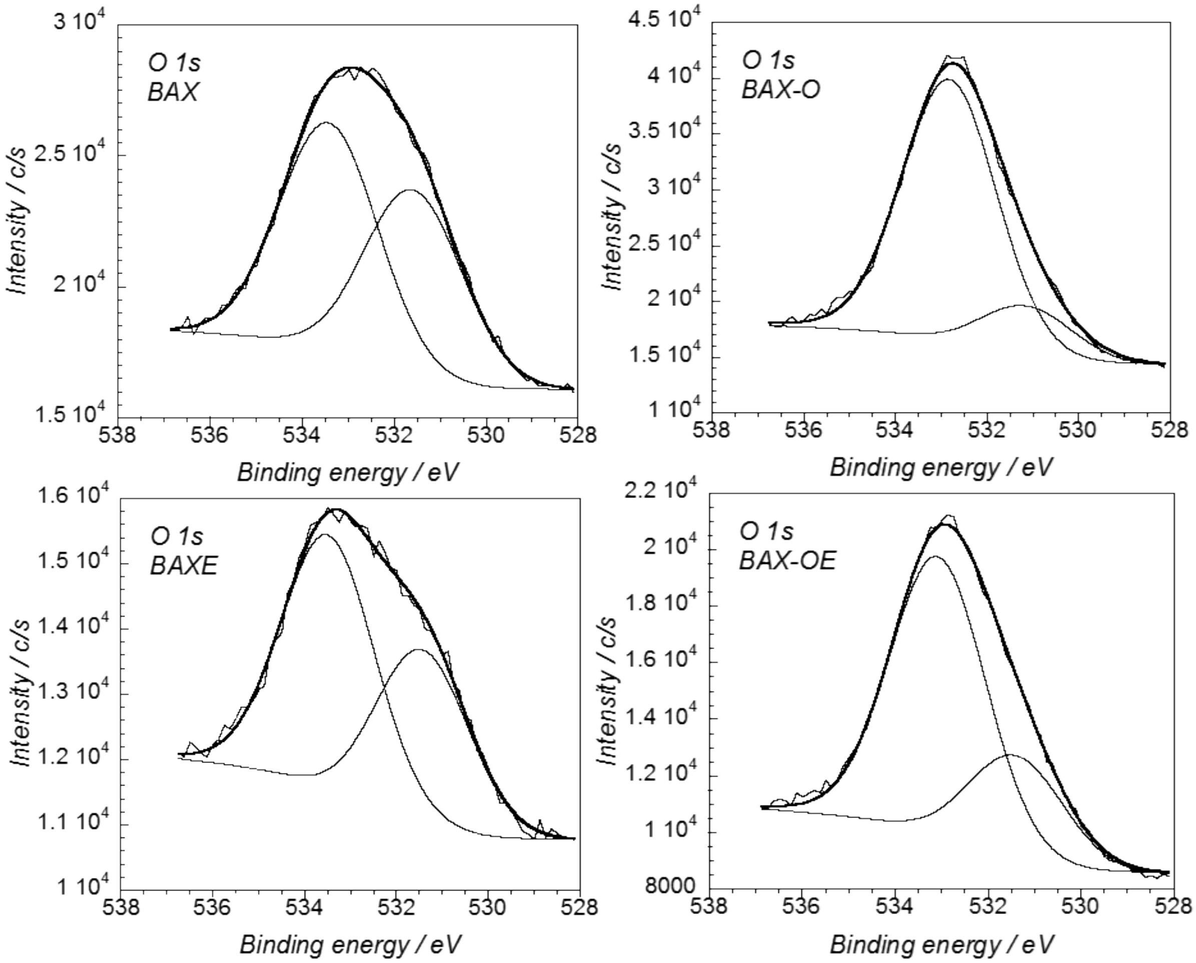

Fig. S6. The deconvolution of O 1*s* core energy levels for the initial and exposed to ammonia carbons.

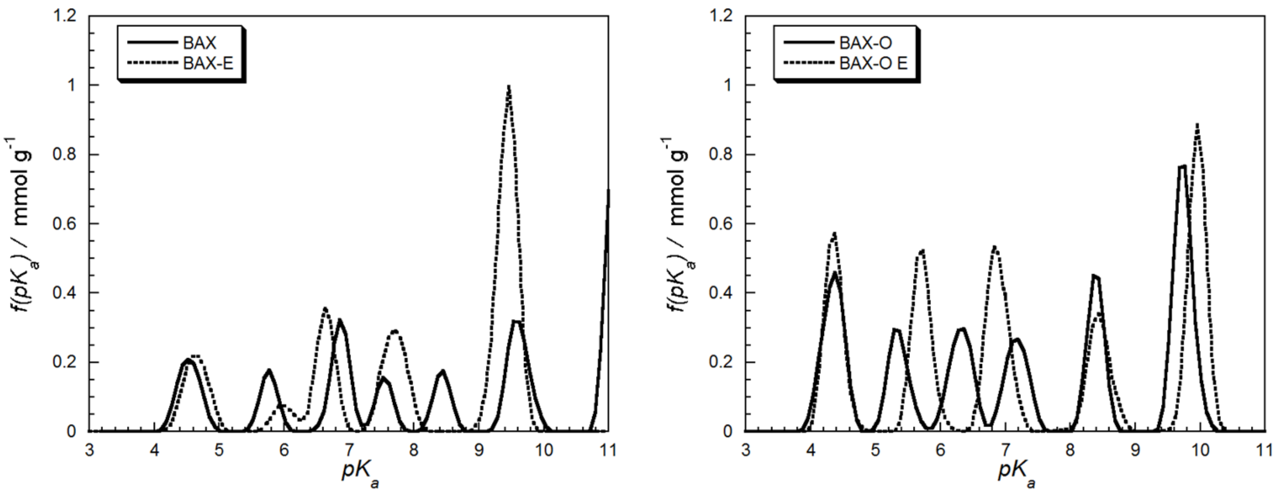

Fig. S7. The distributions of the pK_a for the species present on the carbon surfaces before (A) and after (B) ammonia adsorption.

Detailed information about the surface acidity, which is expected to affect ammonia reactive adsorption, is presented in Fig. S7, where, pK_a distributions are collected. As expected, oxidation of BAX resulted in a significant increase of its acidity. While the total number of acidic groups determined from the potentiometric titration for BAX is 0.276 mmol g^{-1}, after oxidation, this number increased to 0.484 mmol g^{-1} for BAX-O. For the exhausted materials, after ammonia adsorption, the total number of acidic groups determined from the potentiometric titration remain at the same level for BAX-E (0.27 mmol g^{-1}), while for BAX-O E, the number of acidic species increased of about 30 % (0.636 mmol g^{-1}). This might be linked to formation of amines and amides.[1] For BAX, after ammonia adsorption, the number of groups with pK_a 7-8 increase more than twice, which we link to the formation of amines and aminopyridines.[2] This assignment is based the deconvolution of N 1*s* core energy levels, where the content of nitrogen in $C\text{-}NH_2$ groups increases after ammonia adsorption, while the content of nitrogen in pyridine groups decreases, and this could be probably linked to the conversion of some pyridines to aminopyridines.[3,4] Moreover, after ammonia adsorption, BAX exhibits an almost threefold increase in the number of species at pK_a 9-10. This peak is assigned to the formation of NH_4^+ and indicates the formation of ammonium salts produced from the reaction of ammonia with acidic functional groups.

For the exhausted oxidized sample after ammonia adsorption, the increase in the number of groups at pK_a between 4-5, 5-6 and 9-10 is probably attributed to different nitro-type complexes, as suggested by the deconvolution of N 1*s* core energy levels, which showed that the nitrogen content in R-NO_2 and Ph-NO_2 species increases after ammonia adsorption.

References

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