Electronic Supplementary Material (ESI) for Journal of Analytical Atomic Spectrometry.

SUPPLEMENTARY MATERIALS

Multiscale modeling of VOC-graphene nanostructure interactions: designing new sorbents for portable mass spectrometric applications

Stevan Armaković[1,*], Milena Aleksić[2], Stamatios Giannoukos[3], Boris Brkić[2,*]

[1]University of Novi Sad, Faculty of Sciences, Department of Physics, Trg D. Obradovića 4, 21000 Novi Sad, Serbia

[2]BioSense Institute, University of Novi Sad, Dr Zorana Djindjića 1, 21000 Novi Sad, Serbia

[3]Department of Chemistry and Applied Biosciences, ETH Zurich, HCI D 317, Vladimir-Prelog-Weg 3, CH-8093 Zurich, Switzerland

* Corresponance: stevan.armakovic@df.uns.ac.rs ; boris.brkic@biosense.rs

Table S1. Calculated binding energies [kcal/mol] between VOC molecules and modeled sorbents

VOC	GR	GR_O	GR_OH	GR_hole	TENAX
1-propanol	-5.70	-8.86	-11.84	-6.27	-6.55
2-propanol	-5.86	-8.98	-10.37	-6.95	-7.67
acetic-acid	-4.72	-10.82	-14.75	-7.11	-9.07
acetone	-3.92	-9.72	-11.51	-7.72	-7.91
butyric-acid	-7.74	-12.90	-15.49	-9.51	-7.69
ethanol	-4.39	-7.03	-10.50	-5.69	-7.63
isobytiric-acid	-8.18	-13.27	-17.63	-8.45	-11.03
isoprene	-10.40	-11.40	-11.57	-10.36	-9.24
n-pentan	-8.42	-8.28	-9.60	-8.78	-7.38
propionic-acid	-6.54	-12.27	-15.09	-8.19	-9.88

The data from this table was used to generate Figure 5 from the main text.