

Supporting information

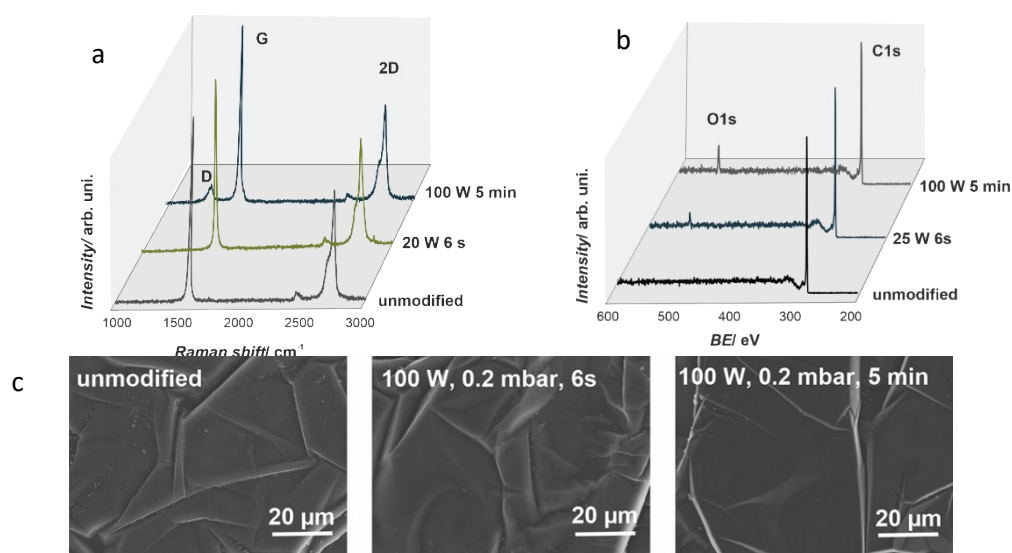
## Functionalization of graphenic surfaces by oxygen plasma toward enhanced wettability and cell adhesion: experiments corroborated by molecular modelling

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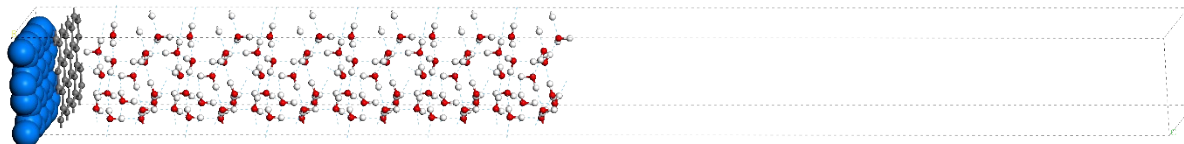
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**Figure S11.** Basic physical-chemical characterization of the investigated graphenic paper in the unmodified and oxygen plasma modified form, a. Raman spectra, b. XPS survey scans and c. SEM images. The results show a comparison between the unmodified and oxygen-functionalized graphenic paper with the use of the most severe plasma treatment parameters (generator power 100 W, exposure time 5 min, oxygen pressure 0.2 mbar). Some of the presented results are adopted from our previously published paper <sup>1</sup>.



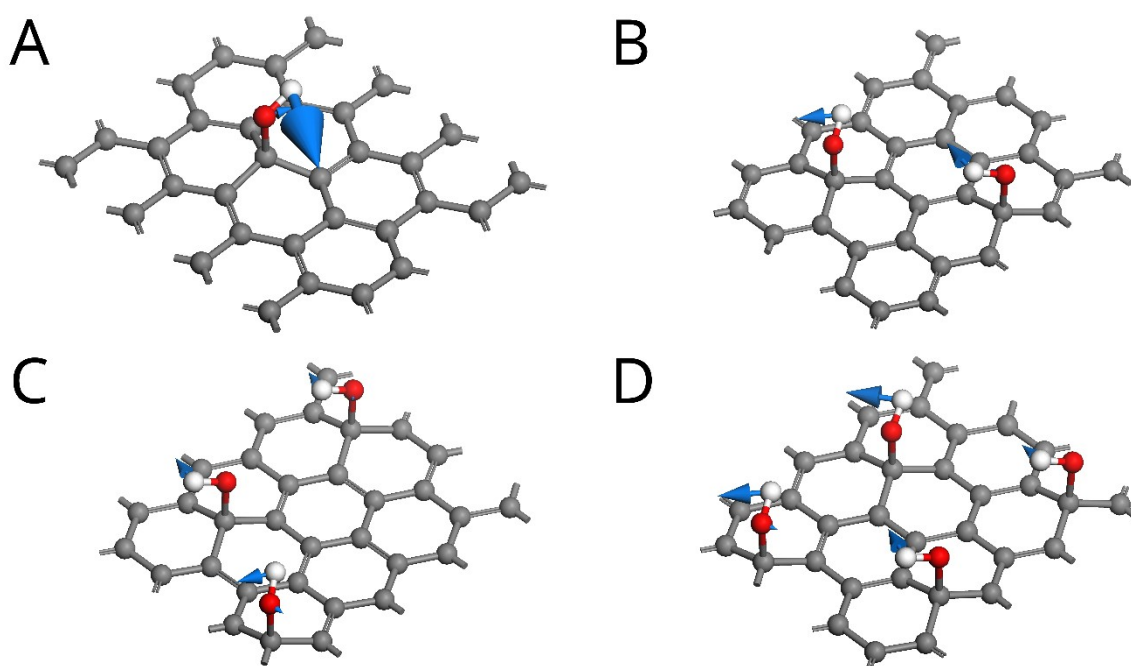
**Figure S12.** A computational model of bare graphene bilayer with adsorbed ice slab. The height of the computational unit cell is equal to 100 Å. Color coding: bottom graphene layer – large blue spheres, top graphene layer - grey, O – red, H - white. Hydrogen bonds are shown as dashed pale blue lines.

**Table S11.** LDI-MS interpretation of the detected functional groups present on the surface of unmodified and oxygen modified graphene.

m/z	formula	probable functional groups
<b>a. unmodified</b>		
648.923	C <sub>54</sub>	-
780.937	C <sub>65</sub>	-
840.944	C <sub>70</sub>	-
912.957	C <sub>76</sub>	-
1044.963	C <sub>87</sub>	-
1176.977	C <sub>98</sub>	-
1321.139	C <sub>110</sub>	-
<b>b. modified 100 W, 6 s</b>		
179.857	C <sub>11</sub> O <sub>3</sub>	-CO
215.826	C <sub>12</sub> O <sub>2</sub> H K <sup>+</sup>	-COOH
263.789	C <sub>18</sub> O <sub>3</sub>	-CO
275.781	C <sub>19</sub> O <sub>3</sub>	-CO
300.927	C <sub>21</sub> O <sub>3</sub> H	-CO and -OH
484.946	C <sub>39</sub> OH	-OH
<b>c. modified 100 W, 5 min</b>		
328.941	C <sub>26</sub> OH	-OH
351.995	C <sub>28</sub> O/C <sub>26</sub> OH Na <sup>+</sup>	-OH/ -CO
393.042	C <sub>30</sub> O <sub>2</sub> H	-COOH
409.012	C <sub>27</sub> H <sub>5</sub> O <sub>5</sub>	-OH
428.975	C <sub>33</sub> O <sub>2</sub> H	-COOH
527.961	C <sub>42</sub> OH Na <sup>+</sup>	-OH

**Table S12** The calculated water contact angle values for the bare surface, and the various –OH and –COOH coverages.

Functionalization (number of groups per 84 Å <sup>2</sup> )	WCA / °
0 (bare bilayer)	89
1 -COOH	45
1 -OH	81
2 -COOH	23
2 -OH	27
4 -COOH	24
4 -OH	22



**Figure S12.** Visualisation of atom position shift (blue arrows) in geometry optimized models of functionalized surface before and after adding ice layer. Gray atoms depict carbon, red denotes oxygen and hydrogen atoms are tinted white. A-D illustrate models with increasing amount of surface groups 1-4 -OH groups, respectively.

## References

- 1 M. Białoruski, D. Kumar, M. Gołda-Cępa, W. Piskorz and A. Kotarba, *Appl Surf Sci*, 2022, **597**, 153671.