Electronic Supplementary Information

New insights into the interactions of phenol with oxygenated functional groups on curved fullerene-like sheets in activated carbon

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Table S1. Comparison of the effects of basis sets: 6-31G(d,p) and 6-311G**. No zero-point energy corrections are applied for these testing calculations.

	Phenol Adsorption Site	Adsorption Energy in Water (kcal/mol) using 6-31G(d,p)	Adsorption Energy in Water (kcal/mol) using 6-311G**
1	Virgin carbon sheet	-27.41	-29.35
2	Carbon sheet with 2×COOH on plane	-27.79	-29.48
8	COOH on carbon sheet	-19.83	-20.09