

Supporting Information Available

An NMR Study of Preferential Endohedral Adsorption of Methanol in Multi-walled carbon nanotubes

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SI-1. TEM image of O-CNTs

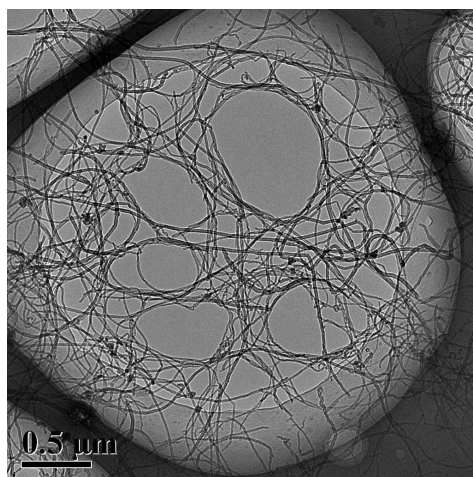


Figure SI. TEM image of O-CNTs after concentrated HNO₃ treatment.

SI-2. ESR spectra of O-CNTs for NMR analysis

EPR measurement was performed at 100 K using a Bruker EMX spectrometer operating at a microwave frequency of 9.813 GHz and a power of 30 mW. As shown in Figure S2, EPR signal for superparamagnetic catalyst particles is absent, indicating that there is almost no residual catalyst in our NMR sample.

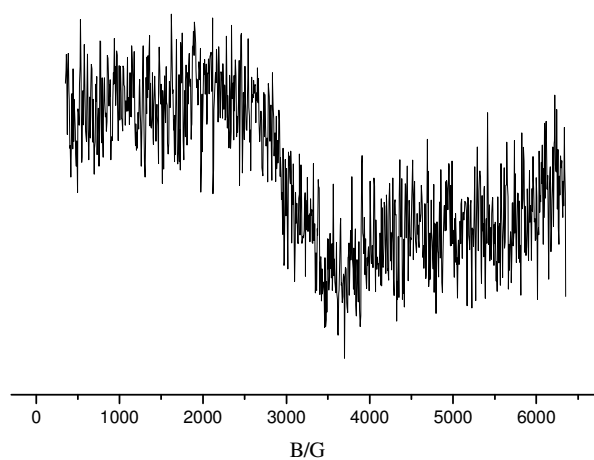


Figure S2. ESR spectrum of O-CNTs after annealing at 1173 K under Ar atmosphere.

SI-3. Computational model for methanol inside and outside (6,6) and (11,0) nanotubes.

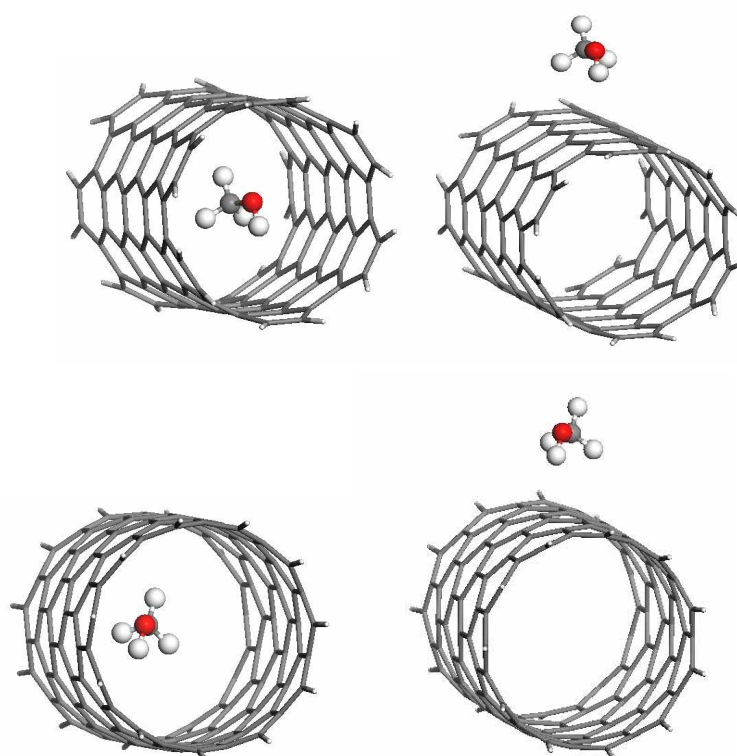


Figure S3. Upper panels and lower panels are optimized structures for methanol inside and outside

(6,6) and (11,0) nanotubes respectively.