Environmentally hazardous gas sensing ability of MoS_2-nanotube: An insight from electronic structure and transport properties

Nabajyoti Baildya*[a], Narendra Nath Ghosh[b] and Asoke P. Chattopadhyay[a]

[a]Department of Chemistry

University of Kalyani, Kalyani 741235, India

[b]Department of Chemistry

University of Gour Banga, Mokdumpur, Malda, 732103, India

Email: nabajyotibaildya@gmail.com, ghosh.naren13@gmail.com, asoke@klyuniv.ac.in

Table S1: Adsorption energies of different gases on MoS_2-NT

System	Energy of gas adsorbed MoS_2-NT at different sites (eV)				Energy of MoS_2-NT (eV)	Energy of gas (eV)	Adsorption energy at different sites (eV)			
	H-site	B-site	M-site	S-site			H-site	B-site	M-site	S-site
MoS_2-NT@CO	-64310.30	-64310.09	-64310.12	-64310.03	-63703.26	-606.60	-0.44	-0.23	-0.26	-0.17
MoS_2-NT@CO_2	-64757.93	-64758.01	-64757.97	-64758.03	-63703.26	-1054.65	-0.02	-0.10	-0.06	-0.12
MoS_2-NT@NH_3	-64031.46	-64031.97	-64032.24	-64031.52	-63703.26	-328.04	-0.16	-0.67	-0.94	-0.22
MoS_2-NT@H_2O	-64181.88	-64182.81	-64183.26	-64182.06	-63703.26	-478.26	-0.36	-1.29	-1.74	-0.54

Table S2: Comparison of adsorption energies of MoS_2-ML and MoS_2-NT

System	Adsorption energy of MoS_2-ML@gas (eV) [1]	Highest adsorption Energy of MoS_2-NT@gas (eV)
MoS_2-NT@CO	-0.0067	-0.44
MoS_2-NT@CO_2	-0.0072	-0.12
MoS_2-NT@NH_3	-0.0100	-0.94
MoS_2-NT@H_2O	-0.0267	-1.74

Table S3: Mulliken charges on MoS_2-NT adsorbed gases

System	Mulliken charges
MoS_2-NT@CO	-0.08e
MoS_2-NT@CO_2	-0.07e
MoS_2-NT@NH_3	0.25e
MoS_2-NT@H_2O	0.08e

References:

[1] S. Zhao, J. Xue, W. Kang, Gas adsorption on MoS2 monolayer from first-principles calculations, Chemical Physics Letters 595 (2014) 35-42.