

# **Electronic Supplementary Information**

**for:**

## **Metal Oxide Adsorption on Fullerene C<sub>60</sub> and its Potential for Adsorption of Pollutant Gases; Density Functional Theory Studies**

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**Table S1** Absolute energies and their ZPE corrected values (in a.u.), of all studied monomers and the most stable complexes, calculated at B97D/6-311G(d,p) level of theory

<b>Structure</b>	<b>E<sub>abs.</sub></b>	<b>E<sub>abs.</sub>+ZPE</b>
NO <sub>2</sub> /C <sub>60</sub>	-2489.896304	-2489.523166
CO/C <sub>60</sub>	-2398.139382	-2397.769755
NO <sub>2</sub>	-205.029111	-205.020572
CO	-113.275020	-113.270159
NO <sub>2</sub> /Cu <sub>2</sub> O	-3562.607076	-3562.593476
NO <sub>2</sub> /ZnO	-2060.310758	-2060.299128
NO <sub>2</sub> /NiO	-1789.119825	-1789.106436
CO/Cu <sub>2</sub> O	-3470.834605	-3470.823389
CO/ZnO	-1968.654358	-1968.642795
CO/NiO	-1697.365321	-1697.353815
Cu <sub>2</sub> O	-3357.470973	-3357.467955
ZnO	-1855.171485	-1855.170149
NiO	-1583.876049	-1583.874315
Cu <sub>2</sub> O/C <sub>60</sub>	-5642.474147	-5642.107002
ZnO/C <sub>60</sub>	-4140.139071	-4139.772875
NiO/C <sub>60</sub>	-3868.943216	-3868.575763
C <sub>60</sub>	-2284.860930	-2284.496922
NO <sub>2</sub> /Cu <sub>2</sub> O/C <sub>60</sub>	-5847.573250	-5847.194380
NO <sub>2</sub> /ZnO/C <sub>60</sub>	-4345.253214	-4344.876550
NO <sub>2</sub> /NiO/C <sub>60</sub>	-4074.057869	-4073.677722
CO/Cu <sub>2</sub> O/C <sub>60</sub>	-5755.813970	-5755.438505
CO/ZnO/C <sub>60</sub>	-4253.443014	-4253.069440
CO/NiO/C <sub>60</sub>	-3982.349337	-3981.972529