Supplementary Materials

Insights into Cis-Amide-Modified Carbon Nanotubes for Selective Purification of CH4 and H2 from Gas Mixtures: A Comparative DFT Study

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Table S1 shows the binding energies calculated using X3LYP functional and associated to the two-point interaction between the chemical groups used as head of the functional group and carbon dioxide.

Table S1. Binding energies referring to the interaction between heads group and CO_2 by using X3LYP functional.

Head Group	Binding Energy (Kcal/mol)
CH_3CSCH_3	1.42
CH_3COCH_3	2.14
CH3COH	2.22
CH_3OCOCH_3	2.28
$HOCH_2CH_2NH_2$	2.49
CH3OCOSH	2.52
CH_3CSOH	3.38
CH_3CSNH_2	3.39
CH_3SOONH_2	3.62
$HCONH_2$	3.67
CH_3COOH	3.79
CH_3OCONH_2	3.83
CH_3CONH_2	3.92

The binding energies evaluated by using X3LYP functional and related to the intermolecular interaction between OEG-head group and CO_2 are reported in Table S2.

Table S2. Binding energies referring to the interaction between OEG-head group and CO_2. Acetate and acetyl amide are used as heads while one, two and three ethylene glycol monomers were considered as the hooks.

Functional group	Binding Energy (kcal/mol)
ethylene glycol -CH_2OCOCH_3	2.21
di-ethylene glycol -CH_2OCOCH_3	2.26
tri-ethylene glycol -CH_2OCOCH_3	2.25
ethylene glycol -CH_2CONH_2	4.18
di- ethylene glycol -CH_2CONH_2	4.17
tri- ethylene glycol -CH_2CONH_2	4.18