**Theoretical studies of methane adsorption on Silica-Kaolinite interface for shale reservoir application**

**Supplementary information**

**Table S1**. The adsorption energy of methane on the silica-kaolinite interface as a function of its number.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **No. of CH4**  **molecules** |  |  |  |  |
| 6 | -2461.411 | -24.251 | -2612.9207 | -1.000 |
| 8 | -2461.411 | -24.251 | -2661.7447 | -0.790 |
| 14 | -2461.411 | -24.251 | -2808.7563 | -0.559 |
| 20 | -2461.411 | -24.251 | -2954.5223 | -0.404 |
| 25 | -2461.411 | -24.251 | -3076.5088 | -0.352 |
| 33 | -2461.411 | -24.251 | -3270.6729 | -0.272 |
| 47 | -2461.411 | -24.251 | -3611.3224 | -0.215 |

The total energy of 4 layers of methane (47 molecules) = -1141.505 eV

Therefore, -24.287 eV

Hence for fourth layer ,