Supporting Information

Structural and electronic properties of iron doped sodium montmorillonite clays: A first principles DFT study

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The XPS quantitative analysis showing the atomic percentages of the elements present in montmorillonite clay and the chemical composition of montmorillonite clay from Southern Clay Products are shown, respectively, in Table S1 and Table S2.

Table S1. XPS quantitative analysis showing the atomic percentages of the elements present in montmorillonite clay†.

| Element | Mt-Na⁺ (at%) |
|---------|-------------|
| Si      | 18.9        |
| Al      | 8.1         |
| O       | 56.2        |
| Na      | 5.0         |
| Fe      | 0.5         |

Table S2. Chemical composition of montmorillonite clay from Southern Clay Products.²

| Components Content | (wt%) |
|--------------------|-------|
| SiO₂               | 67.2  |
| Al₂O₃              | 22.5  |
| Fe₂O₃              | 4.67  |
| Na₂O               | 3.2   |
| MgO                | 2.31  |
The FTIR spectra and the XRD pattern of montmorillonite clay are shown, respectively, in Figure S1 and Figure S2.

**Figure S1.** FTIR spectra of montmorillonite clay.

**Figure S2.** XRD pattern of montmorillonite clay.
Reference

(1) Suzana, A. F. Utilização do método grafiting para obtenção do material híbrido. In Dissertação de Mestrado: Materiais híbridos argila-poli(metil metacrilato) obtidos através do método grafiting; Instituto de Química - Universidade Estadual Paulista: Araraquara, 2015; pp 44.

(2) Angaji, M.; Zinali, A.; Gazvini, N. Study of physical, chemical and morphological alterations of smectite clay upon activation and functionalization via the acid treatment. World J. Nano Sci. Eng. 2013, 3, 161-168, DOI:10.4236/wjnse.2013.34019.