

Electronic Supplementary Information

Interaction of bioactive molecule with surfaces of nanoscale transition metal oxides: experimental and theoretical studies

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Preparation of BTT solution and metal oxide nanoparticles suspension

About 1.5 mg of metal oxide was added in 10 mL of double distilled water and it was dispersed using ultrasonic (LAB MAN, LMUC-12) bath for 1 h. The metal oxides were dispersed completely. The dispersed oxides were used for spectroscopic measurements. BTT solution of strength 0.5 mM was prepared by dissolving 1.1 mg of solid MBT in 10 mL of double distilled water. This BTT solution was needed to further dilute 5 times prior recording the spectra for optimum optical density.

Table S1: Calculated magnetic moment (per atom) for various surfaces

| Surfaces | Magnetic moment (per Fe/Ni atom)(in μB) |
|---|---|
| $\alpha\text{-Fe}_2\text{O}_3(001)$ (O-terminated) | 1.99 |
| $\alpha\text{-Fe}_2\text{O}_3(001)$ (ferryl-terminated) | 1.97 |
| NiO(100) | 0.45 |
| NiO(111) | 0.65 |

Table S2: Comparison of binding energies of BTT molecule on oxygen terminated $\alpha\text{-Fe}_2\text{O}_3(001)$ surface

| Surface | Vacuum layer (with dipole correction)(\AA) | No of layers | Adsorption energy of BTT (eV) |
|---|---|--------------|----------------------------------|
| $\alpha\text{-Fe}_2\text{O}_3(001)$ (O-terminated) | 15 | 10 | -3.90 |
| | 20 | 13 | -3.78 |

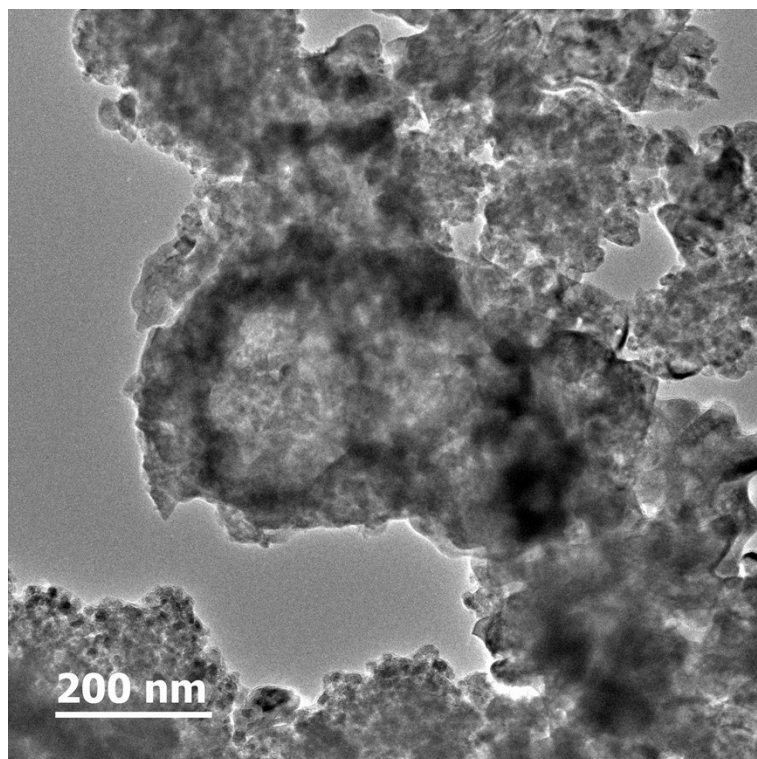


Figure S1: Low resolution TEM image of Fe₂O₃.

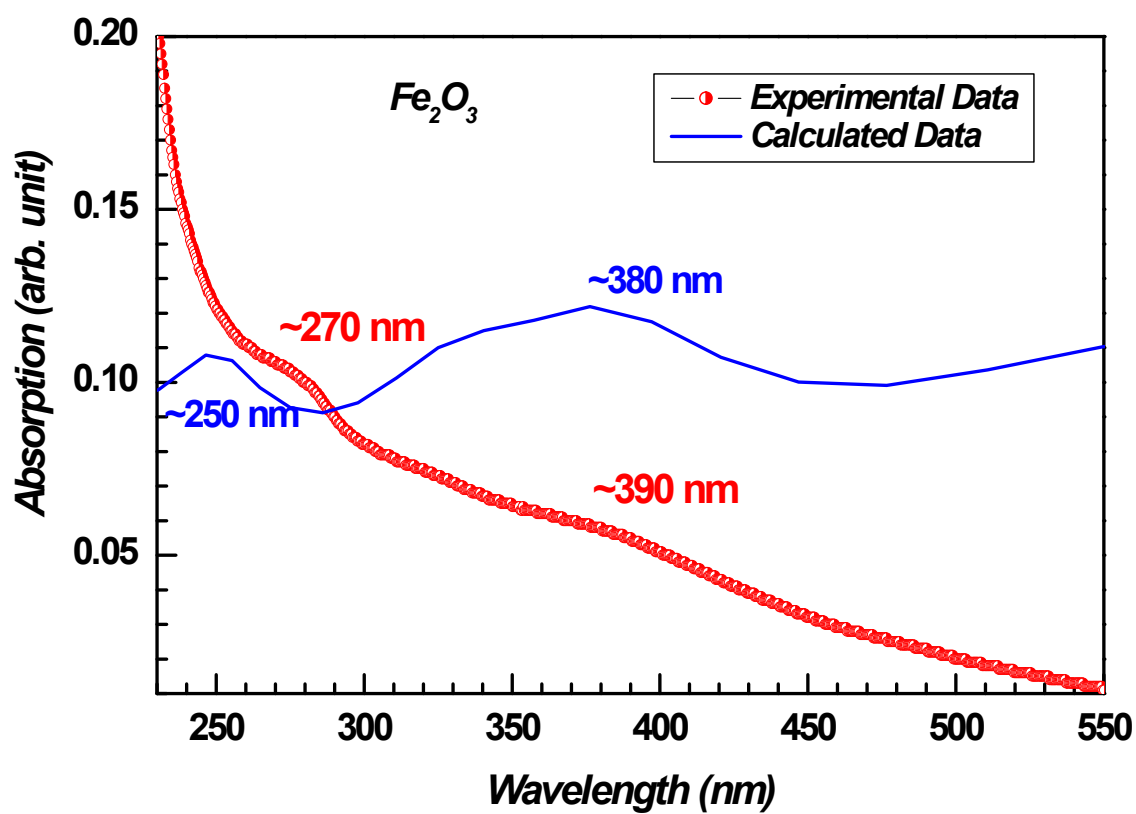


Figure S2: Experimental UV-Vis spectrum of Fe_2O_3 nanoparticles suspended in aqueous medium. The blue line is the theoretically calculated spectrum.

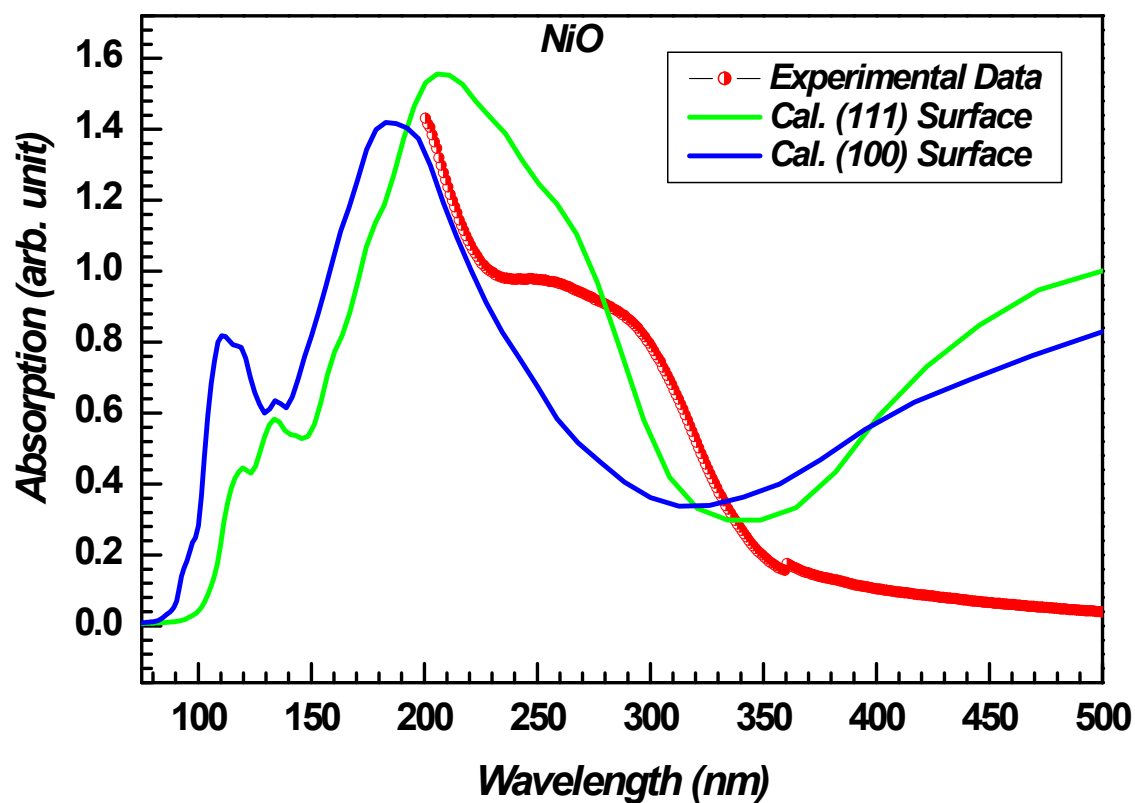


Figure S3: Experimental UV-Vis spectrum of NiO nanoparticles suspended in aqueous medium. The green and blue lines are the theoretically calculated spectrum of NiO on (111) and (100) surfaces, respectively.

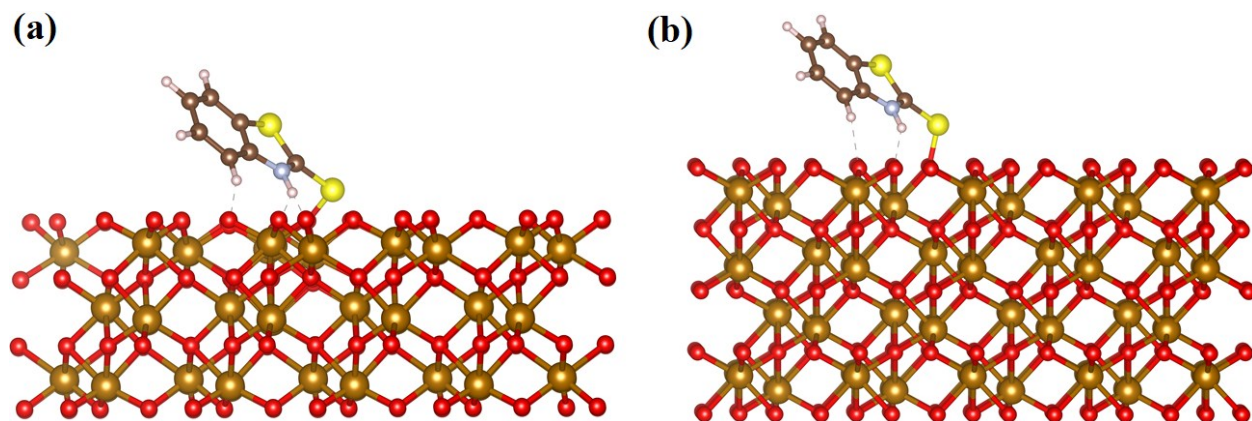


Figure S4: Optimized structures of BTT adsorbed oxygen terminated α -Fe₂O₃(001) surface (a) surface with 10 layers with 15 Å vacuum, (b) surface with 13 layers with 20 Å vacuum.

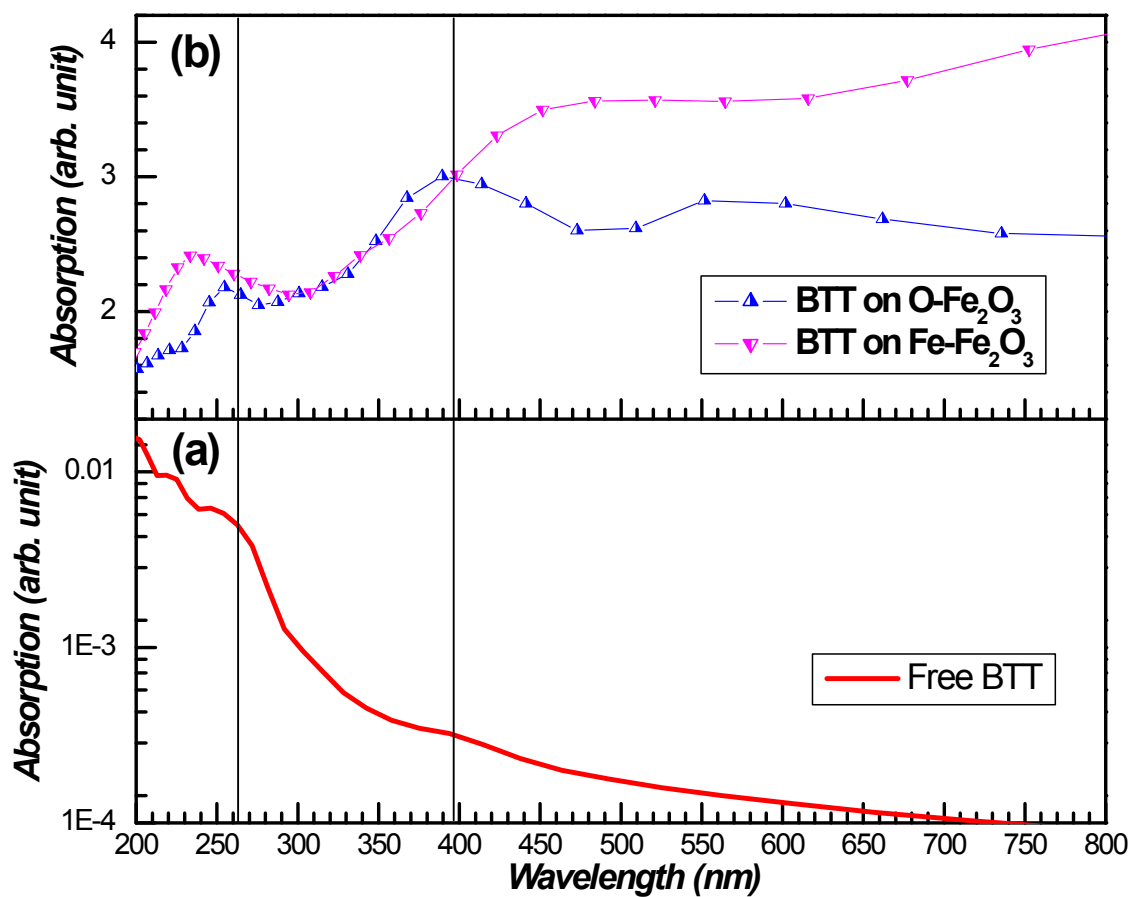


Figure S5: (a) Calculated spectrum of free BTT molecule and (b) BTT attached on O- and Fe-terminated α -Fe₂O₃ surfaces.

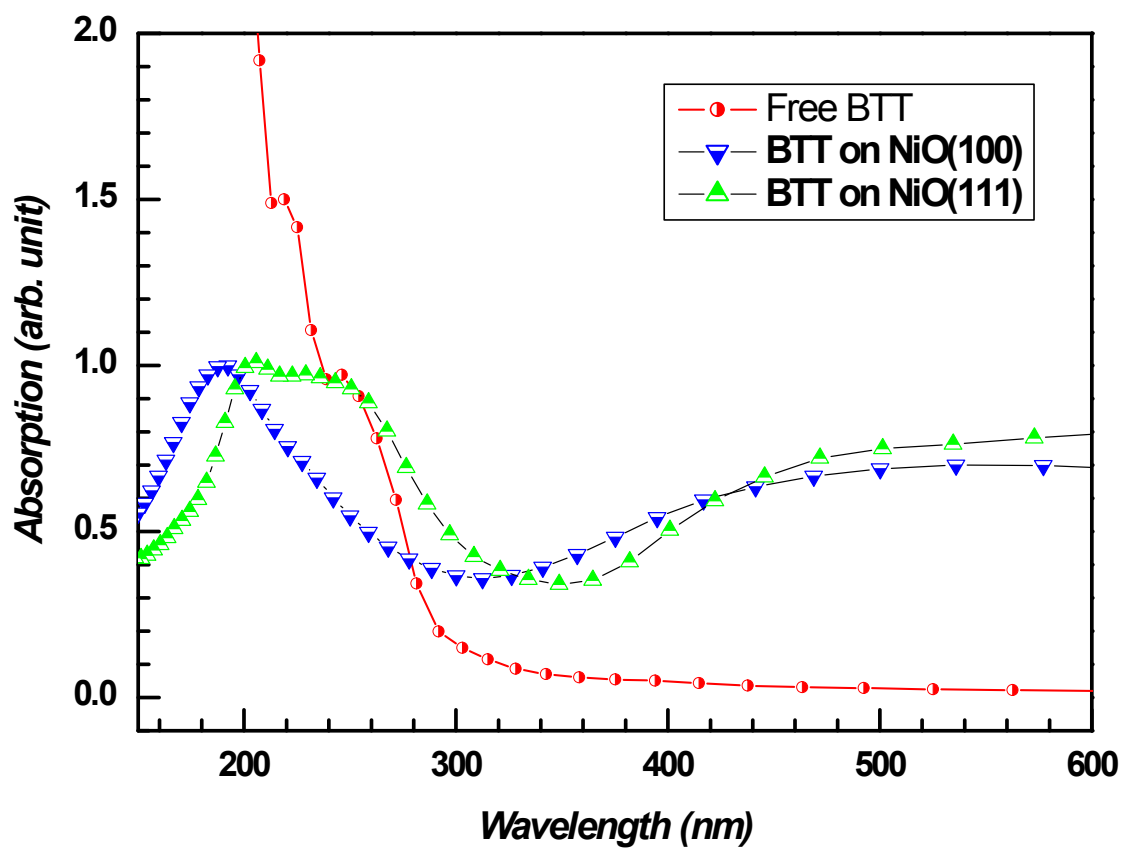


Figure S6: Calculated spectra of free BTT molecule and BTT attached on NiO(100) and NiO(111) surfaces.

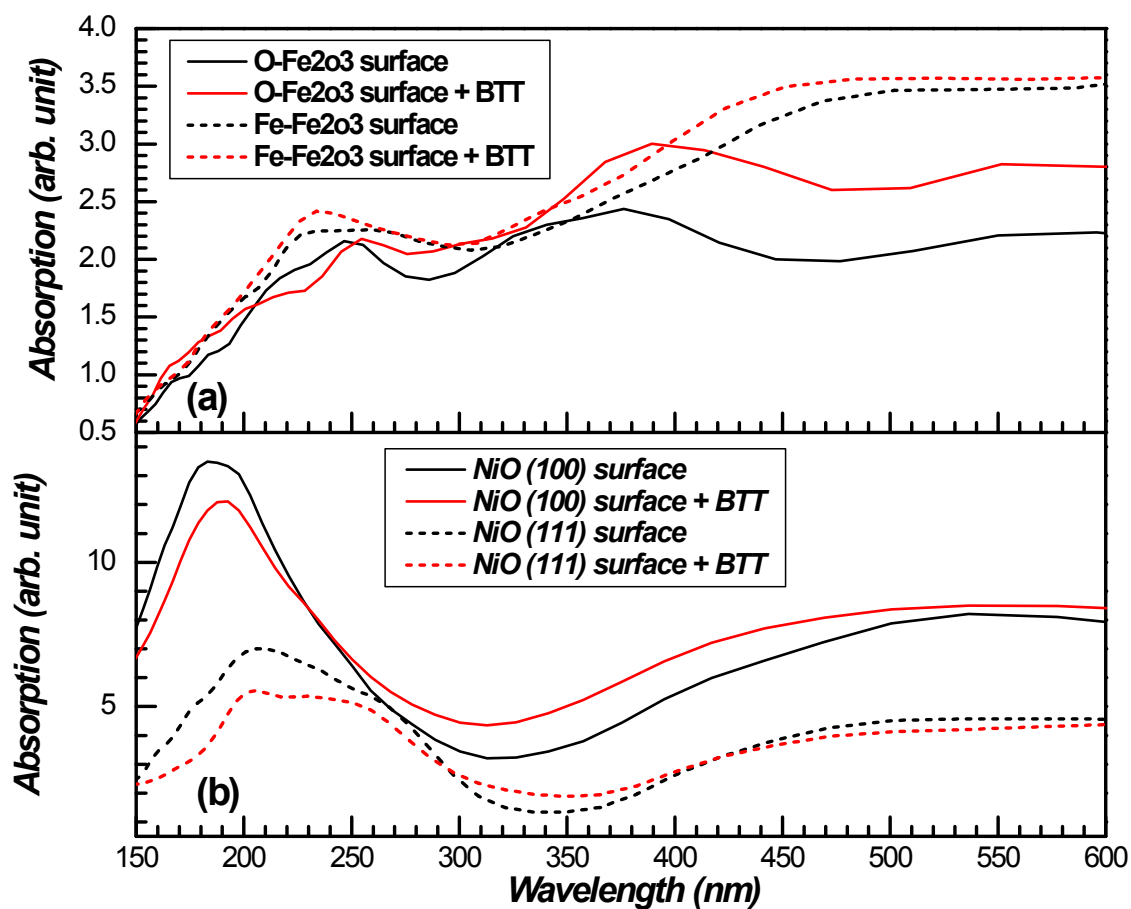


Figure S7: Calculated spectra of free metal surfaces and BTT attached surfaces on (a) α -Fe₂O₃ and on (b) NiO.