

Table S1. Force-field atom types assigned to the constituent atoms of Na<sub>2</sub>Ti<sub>3</sub>O<sub>7</sub>, CoFe<sub>2</sub>O<sub>4</sub>, and Methylene Blue dye used in the Monte Carlo adsorption simulations

Atom	Forcefield type
Na <sub>2</sub> Ti <sub>3</sub> O <sub>7</sub>	
Ti	ti4o
O	o ti
Na	na+
CoFe <sub>2</sub> O <sub>4</sub>	
Co	co2o
Fe	fe2o
O	o fe
Methylene Blue dye	
C (aromatic C–H)	c3a
C (aromatic C–C)	c3a
C (methyl C)	c
C (other methyl C)	c4
N (dimethyl amino)	n3
N (thiazine N)	n2a
H (all hydrogens)	h1