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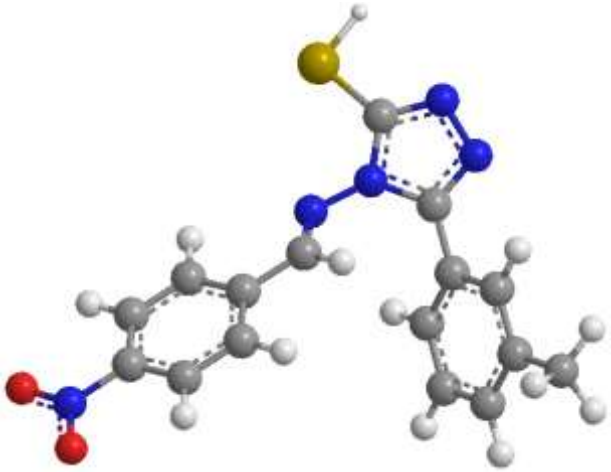
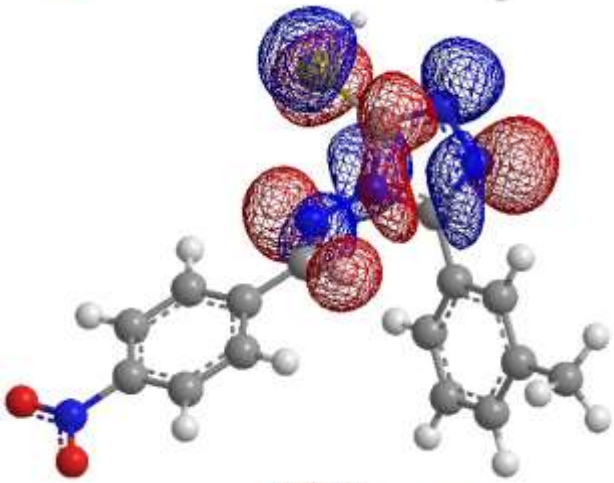
Table S1: Parameters Derived from HOMO and LUMO Calculations

Parameter	Value (eV)	Significance
HOMO	-8.084	**Indicate abilities of inhibitor molecules to donate electrons.** A higher **HOMO energy level** enhances the capability of transferring electron to the metal, facilitating adsorption.
LUMO	-4.552	**Reflects the tendency of molecule for accepting electron.** A lower **LUMO energy level** promotes more effective back-donation from the metal, stabilizing the adsorption process.
HOMO-LUMO Gap (ΔE)	3.532	**A smaller HOMO-LUMO gap signifies increased molecular reactivity,** leading to stronger interactions and improved adsorption on the metal surface.
HOMO-1	-9.311	Indicates additional electron-donating centers that may contribute to adsorption.
LUMO+1	-1.205	Suggests the next available unoccupied orbital, which influences molecular stability.
Electronegativity (χ)	6.318	Indicates capability of inhibitor to draw electron from the metal.
Hardness (η)	1.766	A lower value indicates better inhibition efficiency due to increased reactivity.
Softness (σ = 1/η)	0.566	Higher softness suggests better adsorption and interaction with the metal surface.
Ionization Potential (I = -HOMO)	8.084	Reflects required energy to detach electrons from molecules, signifying its stability.
Electron Affinity (A = -LUMO)	4.552	Demonstrates abilities of inhibitor for receiving electron from the metal.
Fraction of Electron Transfer (ΔN)	0.556	Represents transferring electron from the inhibitor to metal, positive values validate its adsorption potential.

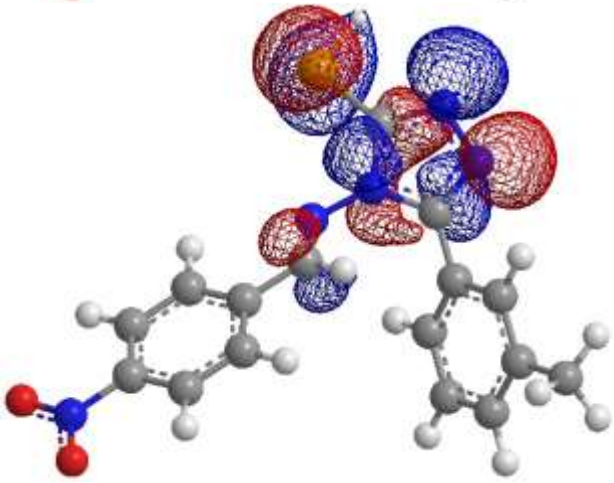
The optimized structure



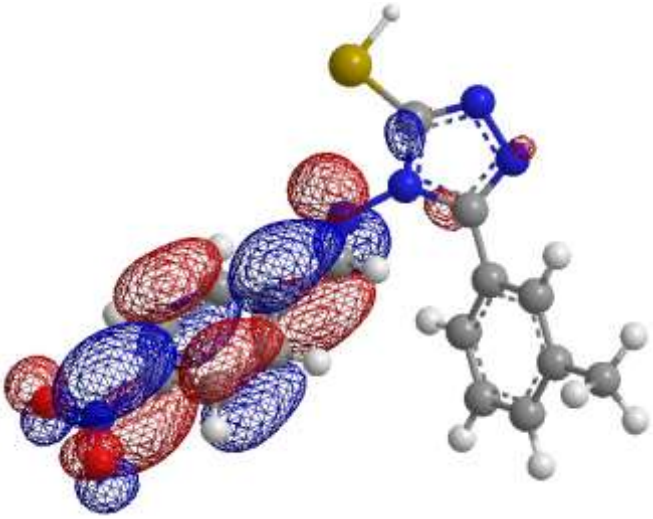
$HOMO$



$HOMO - 1$



$LUMO$



$LUMO + 1$

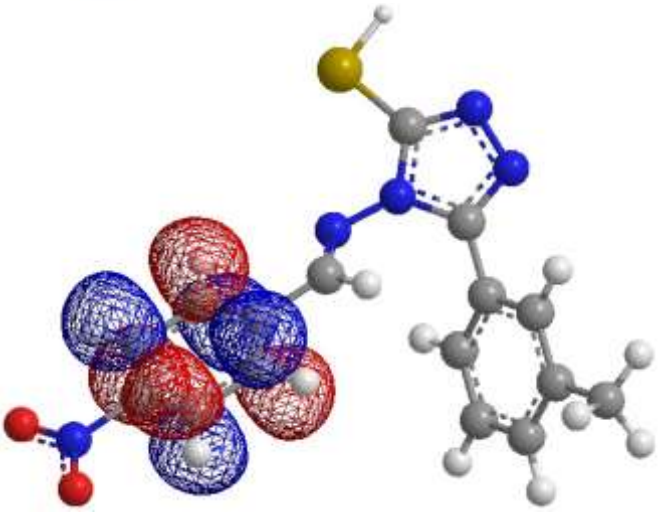


Figure S1. The optimized structure, HOMO, HOMO-1, LUMO+1 and LUMO for MNATT

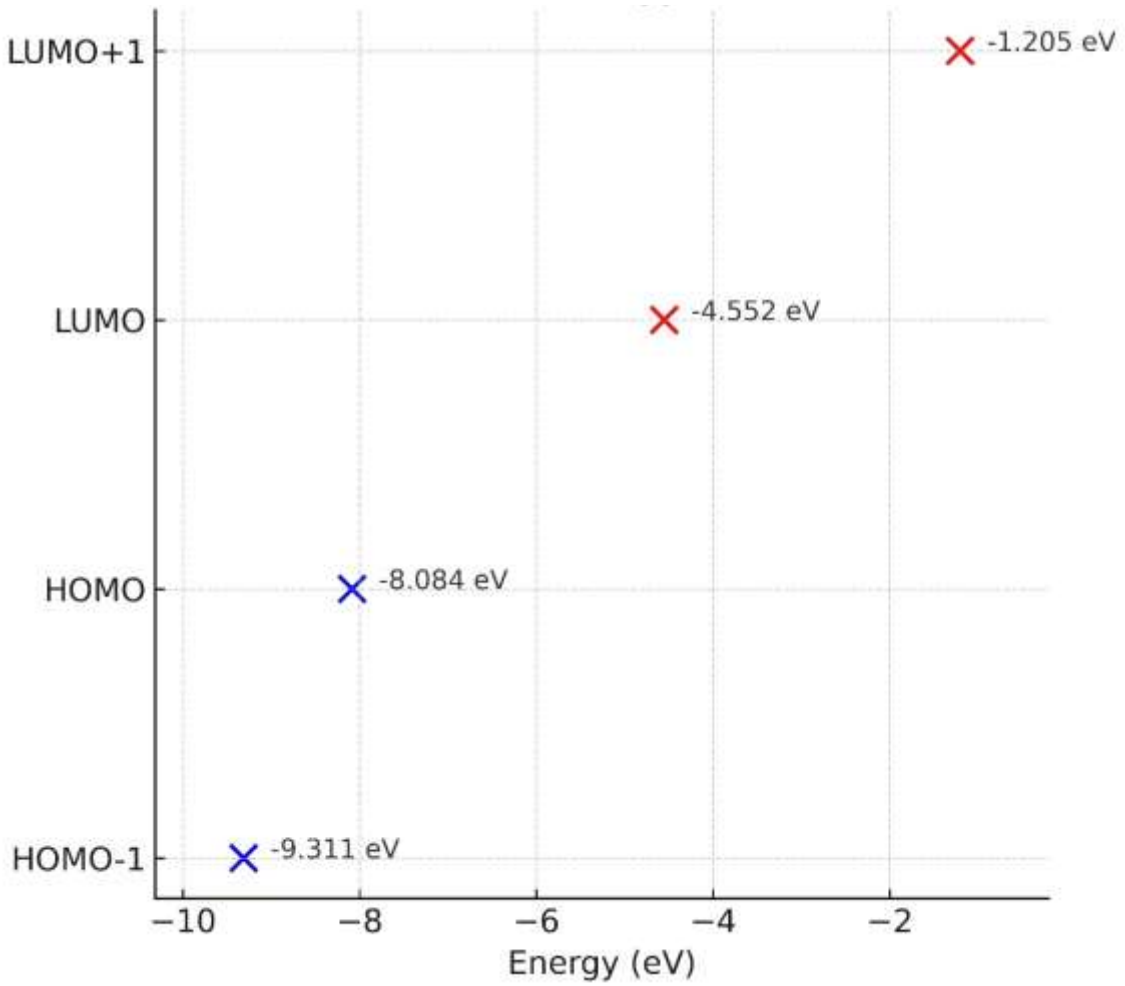


Figure S2: Molecular Orbital Energy Levels of MNATT Derived from DFT Calculations