

Supporting Information

Fabrication of a Highly Tunable Graphene Oxide Composite through Layer-by-Layer Assembly of Highly Crystalline Polyaniline Nanofibers and Green Corrosion Inhibitors: Complementary Experimental and First-Principles Quantum Mechanics Modeling Approaches

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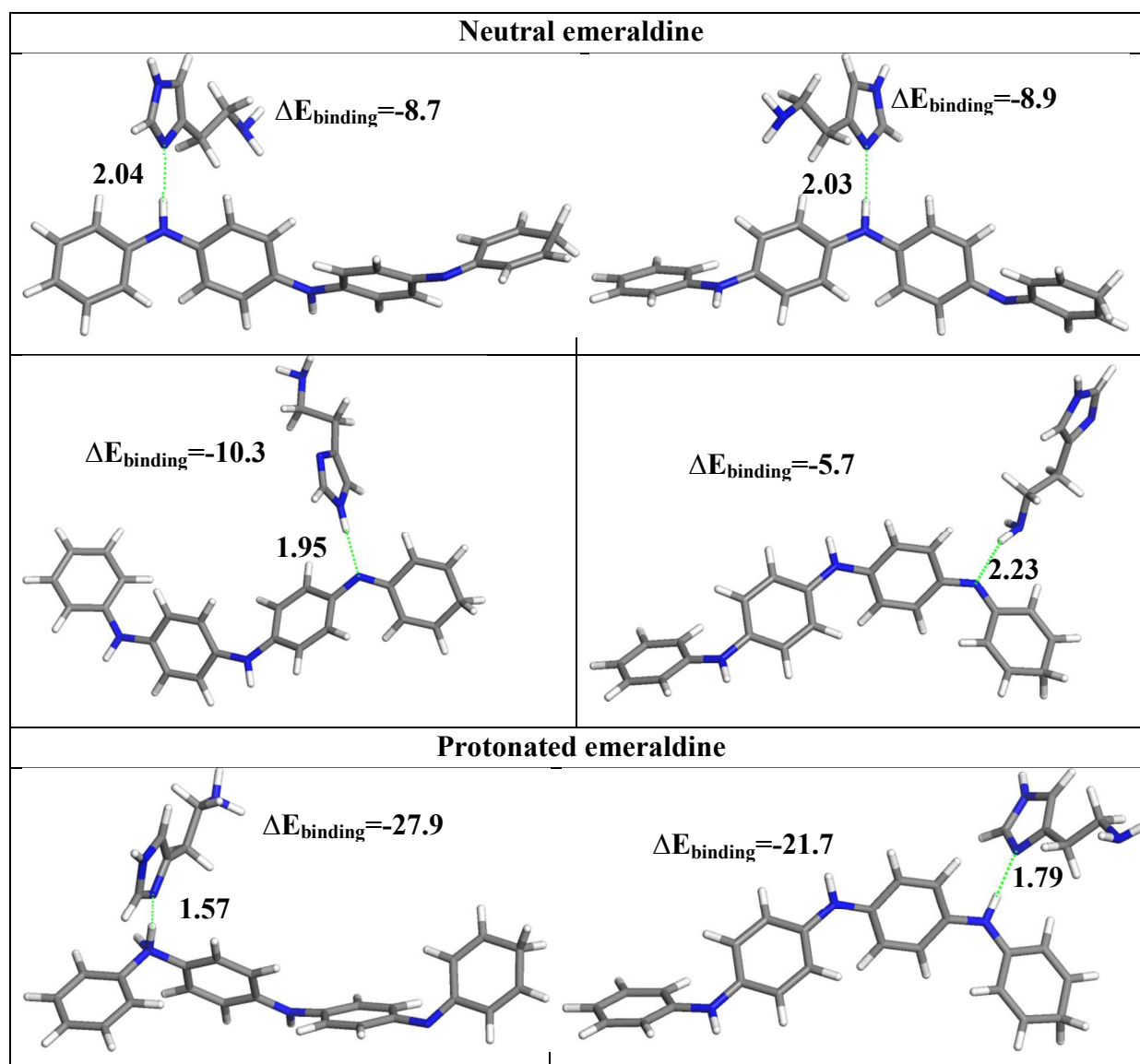


Figure S1- The B3LYP/6-31G(d,p) optimized hystamine interacting with phenyl-terminated neutral/protonated emeraldine trimer form of polyaniline. The calculated binding energies are in kcal/mol, and the H-bonds are in angstrom (Å). The binding energies and H-bond length for nitrogen-terminated emeraldine are shown in parentheses.