147d Design of Corrosion Inhibitors for Carbon Steel Materials Using a Combined Density Functional Theory - Green's Function Approach

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Abstract A new approach which combines the density functional theory (DFT) and Green's function theory is used to study the interaction and electron transfer between the carbon steel materials and the corrosion inhibitors in an attempt to design new environment friendly imidazoline type corrosion inhibitors. The results from DFT calculation for both the inhibitor and carbon steel materials are used as the input of the Green's function electron transfer approach. The DFT is used to calculate the isolated inhibitors, the extend inhibitor molecules consisting of the inhibitor and few iron atoms, as well as the carbon steel material with periodic boundary conditions (PBC). The results from the PBC calculation are used to construct the self-energy terms for the Green's function. The Green's function calculation, the density of states (DOS) of the complex system (inhibitor plus steel substrate) and the electron transmission function between inhibitor and substrate are obtained. This information is then used to guide the rational design of corrosion inhibitors.

Keywords: DFT, Green's function, corrosion inhibitor, carbon iron steel, anticorrosive