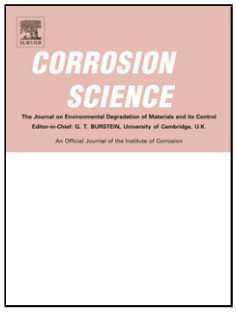

Title: Correlating electronic structure with corrosion inhibition potentiality of some bis-benzimidazole derivatives for mild steel in hydrochloric acid: combined experimental and theoretical studies

Author: Alokdut Dutta Sourav Kr. Saha Priyabrata Banerjee Dipankar Sukul

PII: S0010-938X(15)00266-8
DOI: http://dx.doi.org/doi:10.1016/j.corsci.2015.05.065
Reference: CS 6352

To appear in:

Received date: 21-12-2014
Revised date: 26-5-2015
Accepted date: 27-5-2015

Please cite this article as: A. Dutta, S.Kr. Saha, P. Banerjee, D. Sukul, Correlating electronic structure with corrosion inhibition potentiality of some bis-benzimidazole derivatives for mild steel in hydrochloric acid: combined experimental and theoretical studies, *Corrosion Science* (2015), http://dx.doi.org/10.1016/j.corsci.2015.05.065

Highlights:

- Bis-benzimidazole derivatives as good corrosion inhibitors for mild steel in acid.
- Simultaneous both way electron- transfer is expected to occur during adsorption.
- Role of molecular conformation on inhibition efficiency is demonstrated.
- Good correlation between inhibition efficiency and molecular parameters established.
- MD simulation results support experimental observations.