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

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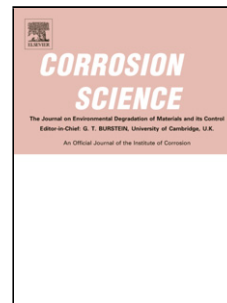
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Highlights:

- 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.

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