

Supplementary materials

Molecular Assembly between Weak Crosslinking Cyclodextrin Polymer and *trans*-Cinnamaldehyde for Corrosion Inhibition towards Mild Steel in 3.5% NaCl Solution: Experimental and Theoretical Studies

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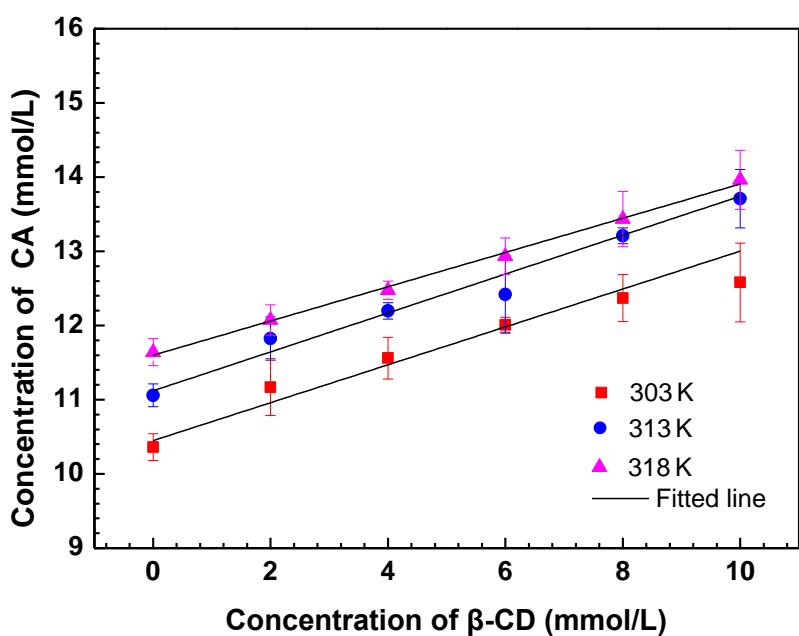


Figure S1. Phase solubility curves of *trans*-cinnamaldehyde with β -cyclodextrin at 303, 313 and 318 K.

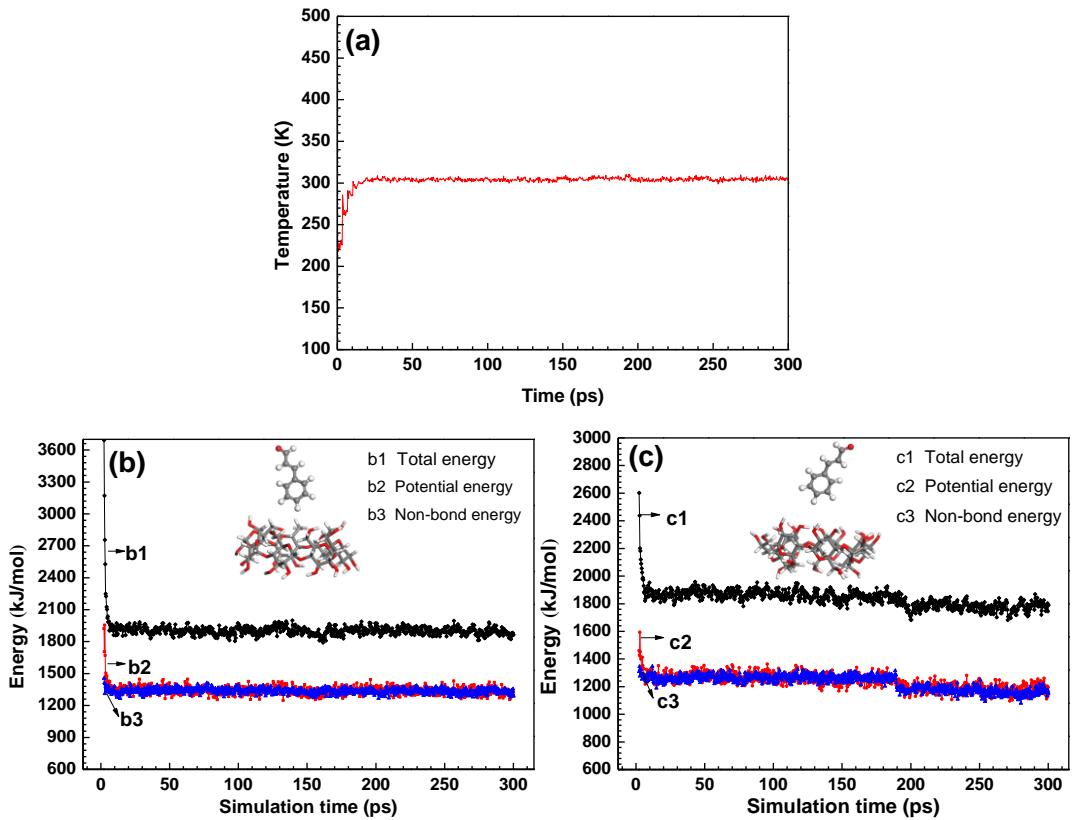


Figure S2. Fluctuations of (a) temperature and (b) energies for *trans*-cinnamaldehyde assembled with β -cyclodextrin through the narrow rim and wide rim during molecular dynamics simulation.

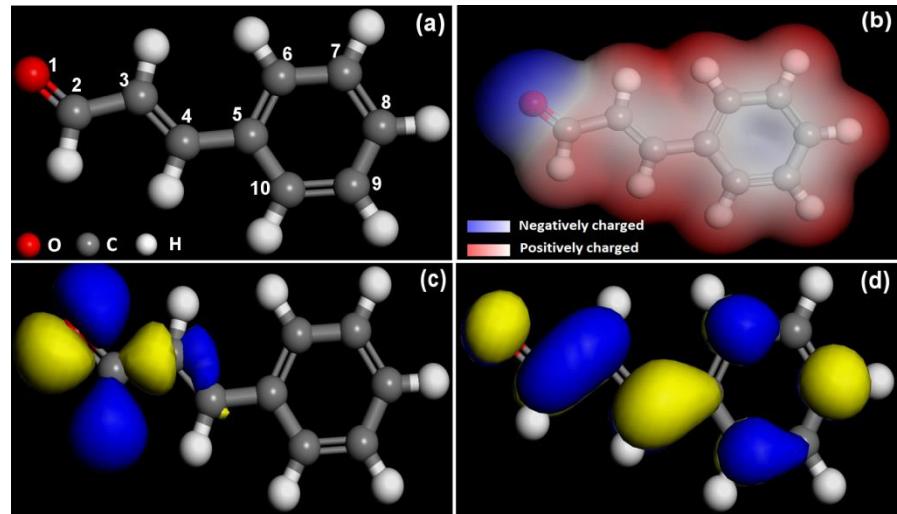


Figure S3. Quantum chemistry descriptors of guest molecule (*trans*-cinnamaldehyde): (a) optimal configuration, (b) mapping of molecular electrostatic potential, (c) HOMO and (d) LUMO distributions.

Table S1. Main composition of Q235A mild steel obtained from optical emission spectroscopy.

| Element | C | Mn | Si | S | P | Fe |
|---------------|------|-----|-----|------|------|---------|
| Content (wt%) | 0.16 | 0.5 | 0.3 | 0.05 | 0.05 | balance |

Table S2. Apparent stability constants and thermodynamic parameters of β -cyclodextrin/*trans*-cinnamaldehyde inclusion complex.

| Temperature (K) | K_s (mol ⁻¹) | ΔH_a (J/mol) | ΔS_a (J/(mol·K)) | ΔG_a (J/mol) |
|-----------------|----------------------------|----------------------|--------------------------|----------------------|
| 303 | 34.3 | | | 8954.8 |
| 313 | 31.1 | -14054.2 | -16.8 | — |
| 318 | 25.8 | | | — |