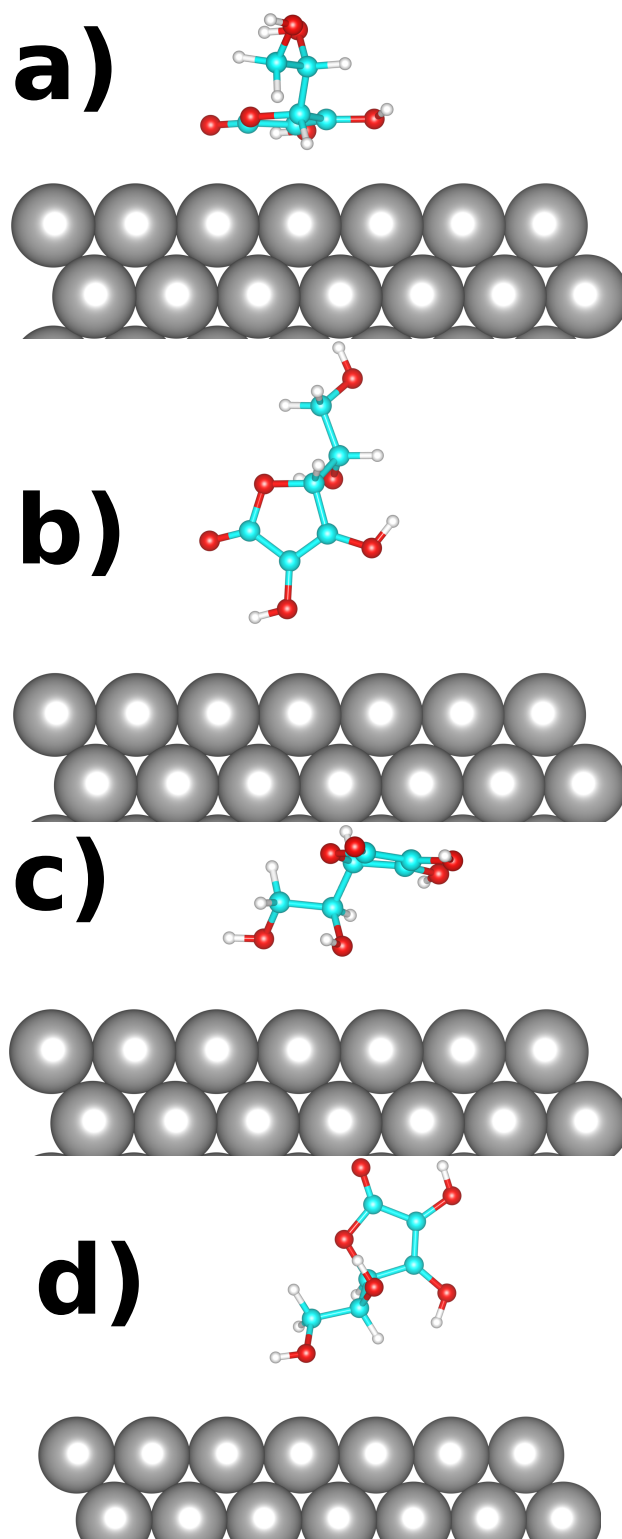
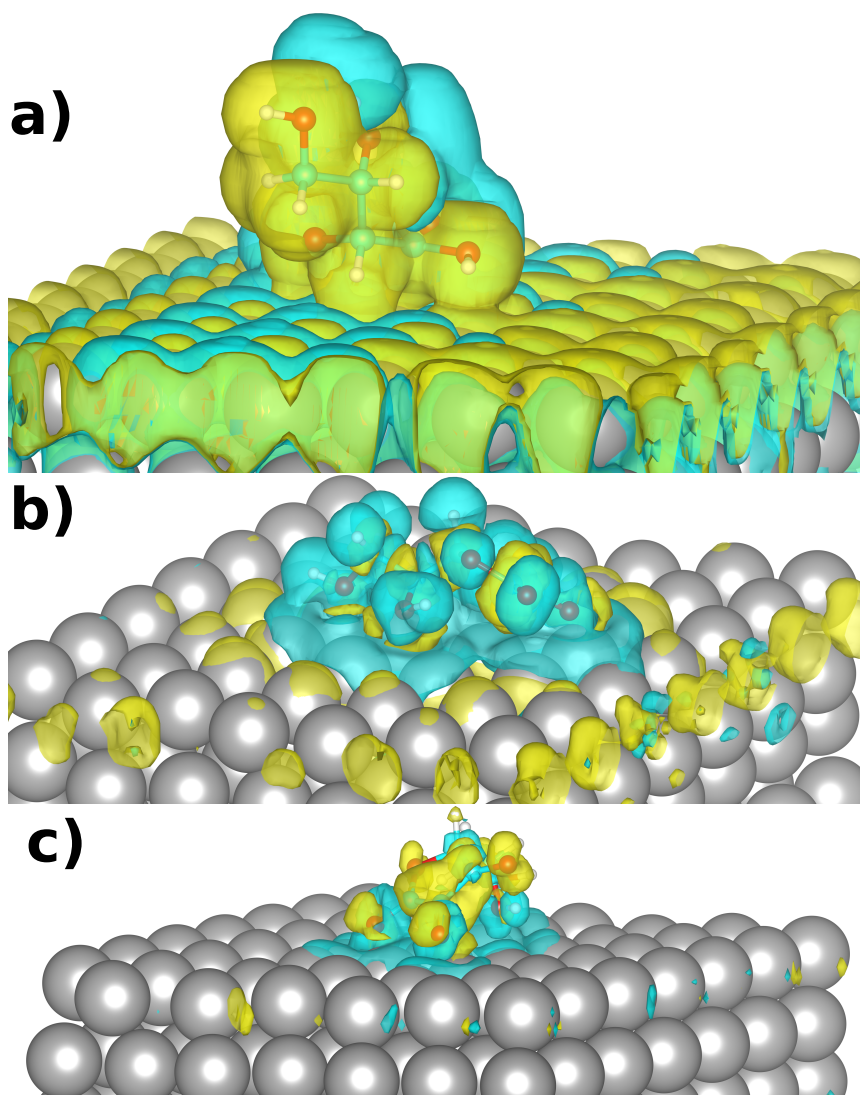


# Supplementary Materials: Ascorbic acid, ascorbate, and dehydroascorbic acid as green corrosion inhibitors: A computational investigation

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**Figure S1.** Initial AA adsorbed structures with perpendicular (figs. b) and d)) and parallel (figs. a) and c)) arrangements on a (110)  $\alpha$ -Fe(110) surface. The same configurations are used for systems containing ASA and DHA as adsorbates.



**Figure S2.** Charge density difference maps of a) AA, b) ASA, and c) DHA on  $\alpha$ -Fe(110) surface in their most stable adsorption configurations.