

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

Bruno D. F. Souza ¹ , Mateus R. Lage ², Adenilson Oliveira dos Santos ², Francisco Ferreira da Sousa ³, Rodrigo Gester ⁴, Stanislav R. Stoyanov ^{5,*}, and Tarciso Andrade-Filho ^{4,*}

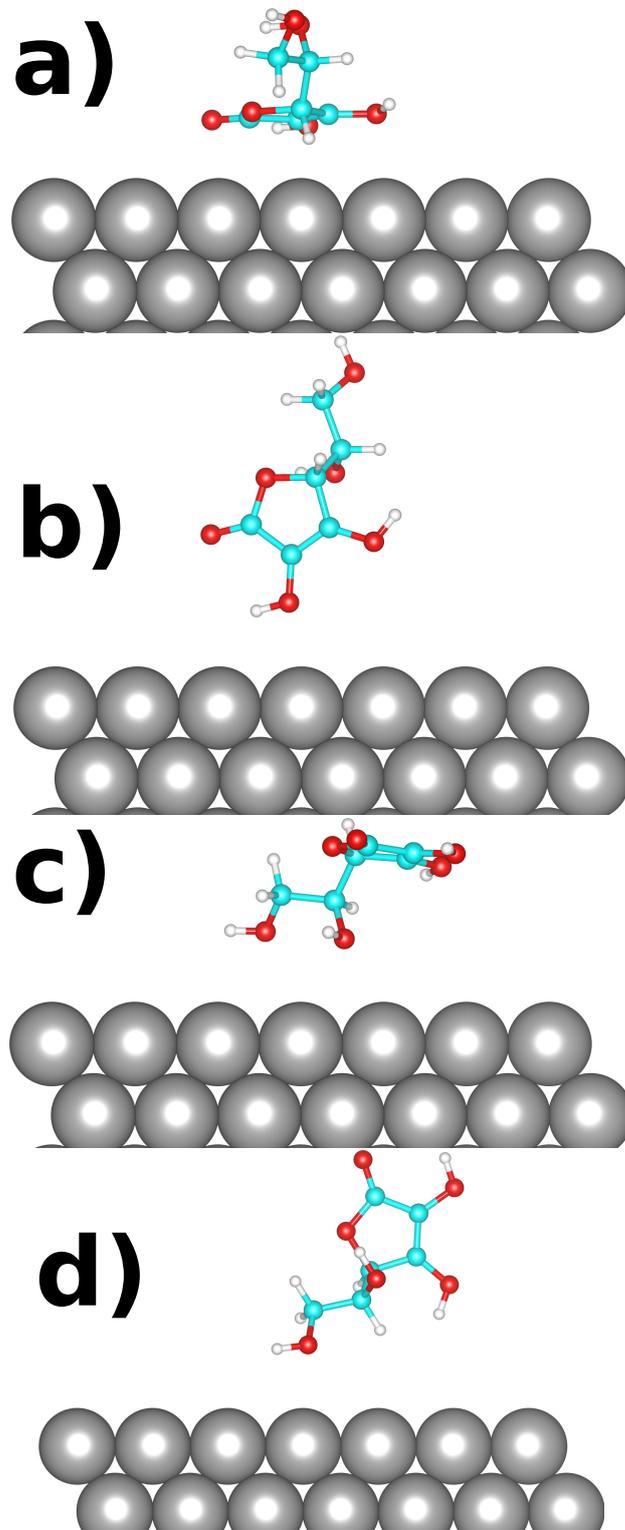


Figure S1. Initial AA adsorbed structures with perpendicular (figs. b) and d)) and parallel (figs. a) and c)) arrangements on a (110) α -Fe(110) surface. The same configurations are used for systems containing ASA and DHA as adsorbates.

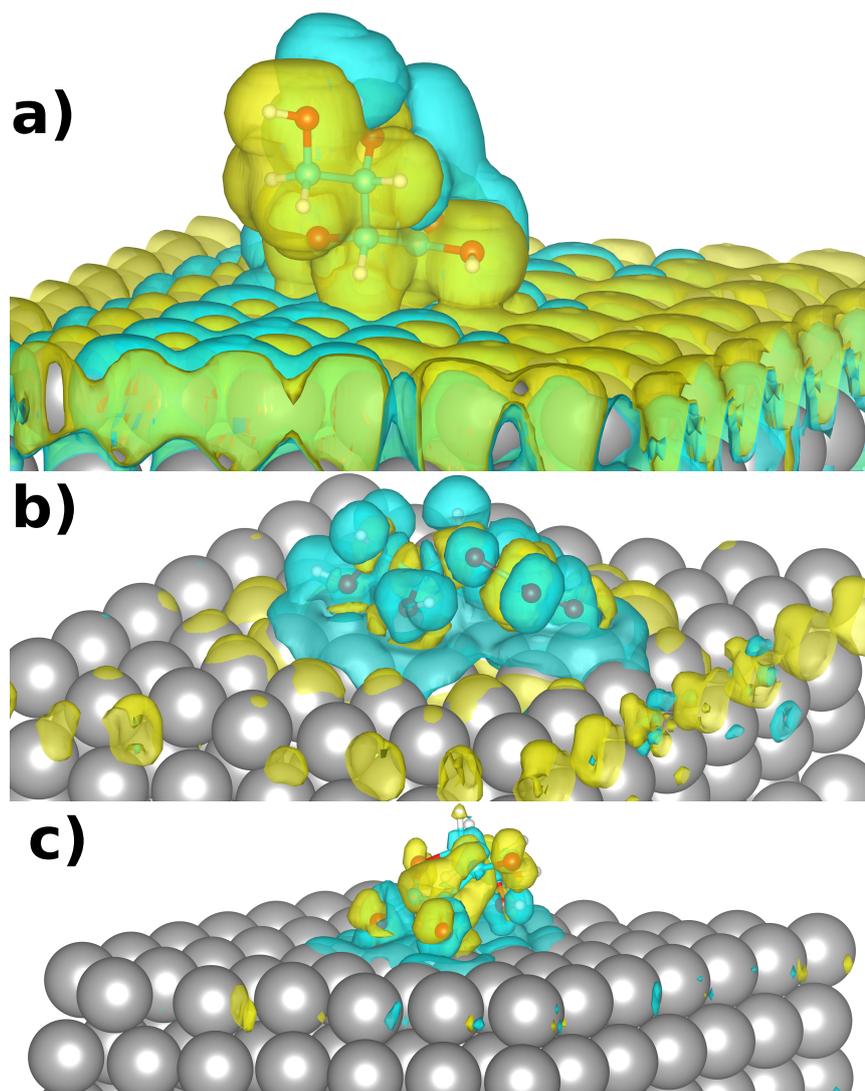


Figure S2. Charge density difference maps of a) AA, b) ASA, and c) DHA on α -Fe(110) surface in their most stable adsorption configurations.