

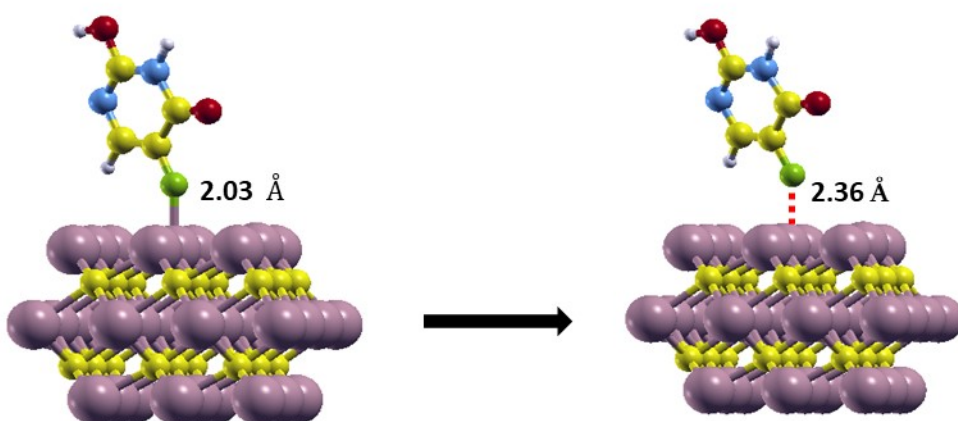
Supplementary material for:

Ti_3C_2 MXene Nanosheets as Novel Drug Delivery for 5-Fluorouracil Anticancer Drug: An Intuition from DFT

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a) Ketoenol (\perp_{Ti1})



b) Ketoenol (\perp_{Ti2})

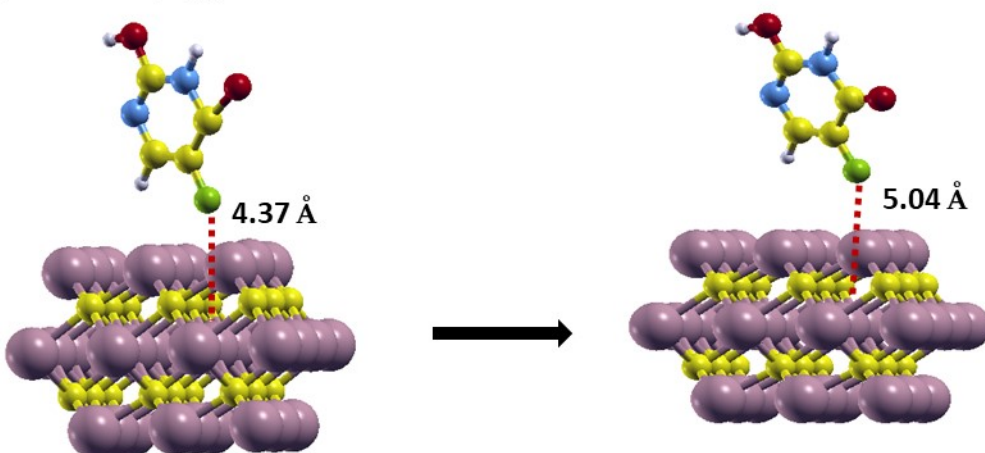
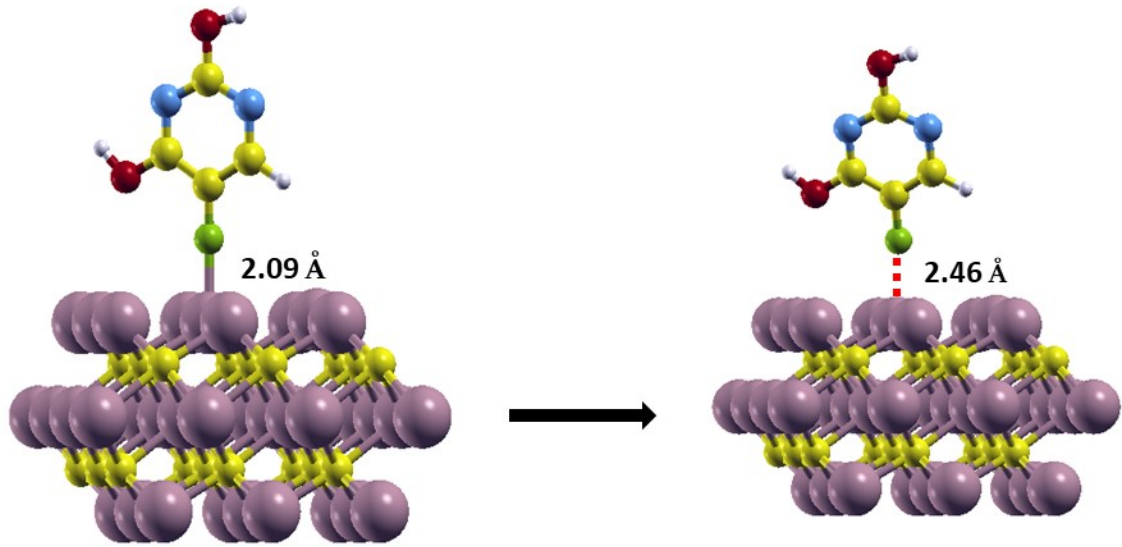


Fig.1.S: Ti_3C_2 @Ketonel at , a) \perp_{Ti1} and b) \perp_{Ti2} configuration before (left) and after (right) the adsorption process

a) Dienol (\perp_{Ti1})



b) Dienol (\perp_c)

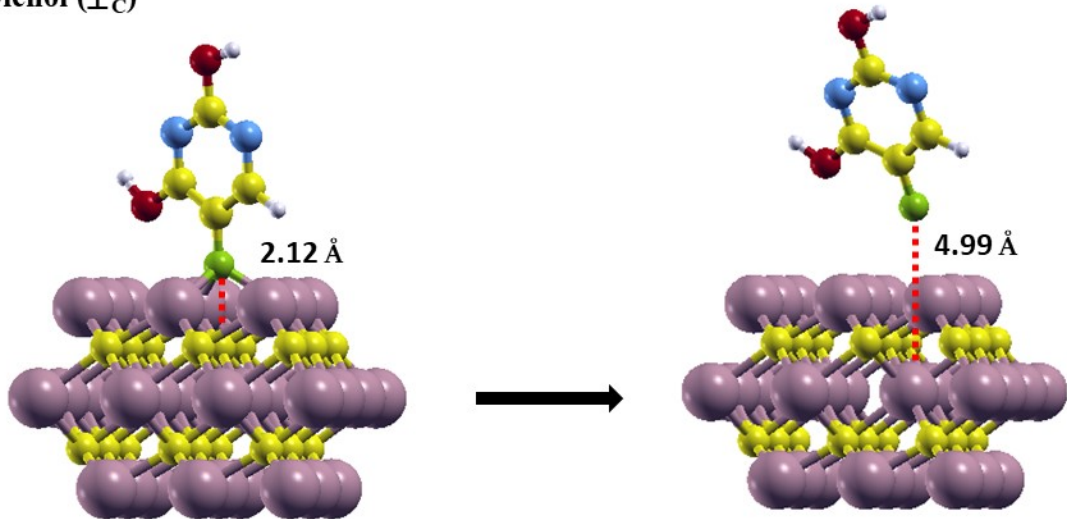
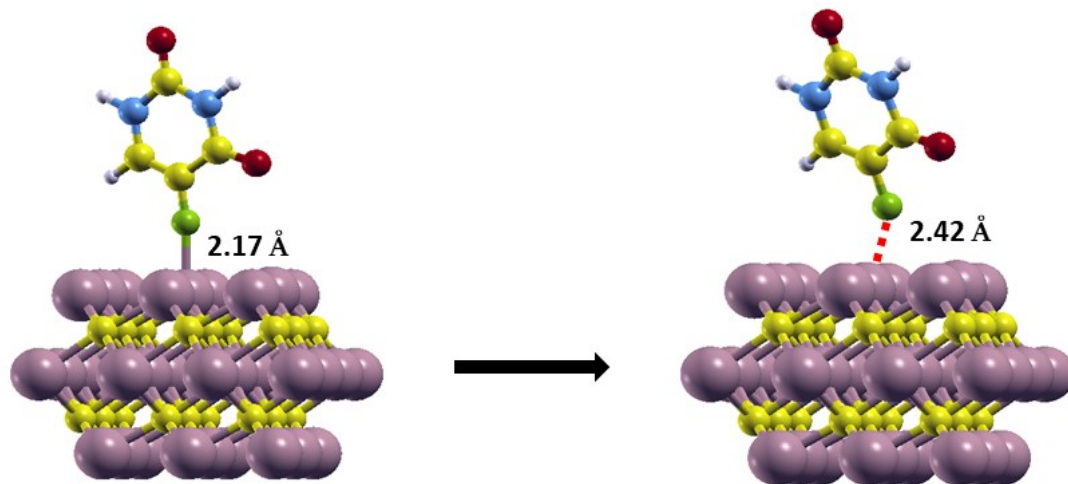


Fig.2.S:Ti₃C₂@Dienol at a) \perp_{Ti1} and b) \perp_c configuration before (left) and after (right) the adsorption process

a) Diketo (\perp_{Ti1})



b) Diketo (\perp_{Ti2})

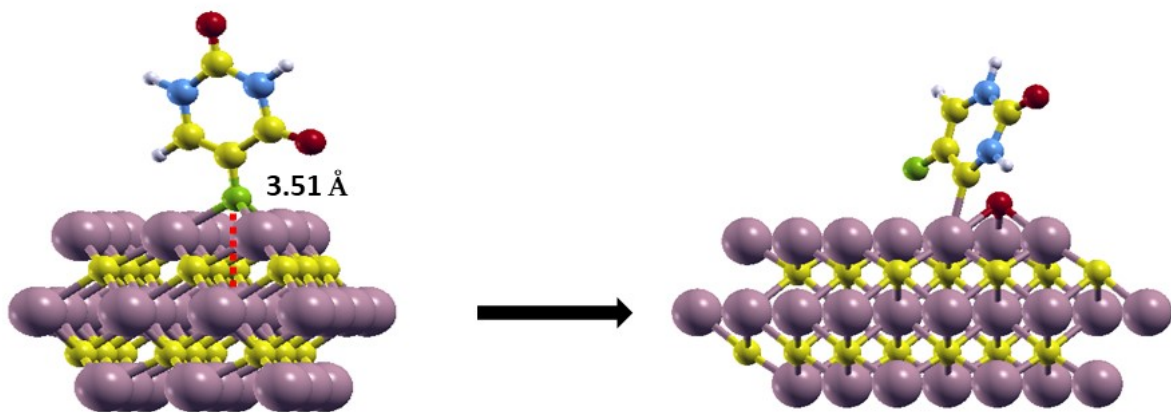


Fig.3.S:Ti₃C₂@Diketo at a) \perp_{Ti1} and b) \perp_{Ti2} configuration before (left) and after (right) the adsorption process