Defluorination and Adsorption of Tetrafluoroethylene (TFE) on TiO_2(110) and Cr_3O_3(0001)

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The capability to join dissimilar materials (cf., e.g., [1-4] and references therein) is a key enabling technology that allows design engineers to create new structures or parts with tailor engineered properties (e.g., a material with high temperature resistance in one area and good corrosion resistance in another). Some notable examples include polymer-metal composites used in various specialized applications (cf., eg., [1,2] and references therein). All of these applications fundamentally start with polymer adhesion on metal surfaces. Recently, we report that metal oxide surfaces catalyze the formation of intermediate defuorinated tetrafuoroethylene (TFE) radicals, resulting in enhanced binding on the corresponding metal oxide surfaces (cf., Fig. 1 [5]). As expected, reactivity of the corresponding metal oxide surfaces depends on the oxygen coordination of metal surface atoms. Thus, introducing oxygen vacancies and non-ionizing radiations to form intermediate radicals could promote binding of polymers to metals and metal-oxide surfaces, allowing for better materials design. This could find significant applications not only in joining dissimilar materials, but also allow for flexibilities in realizing materials with the desired (pre-determined) characteristic properties. Further details will be presented at the meeting.

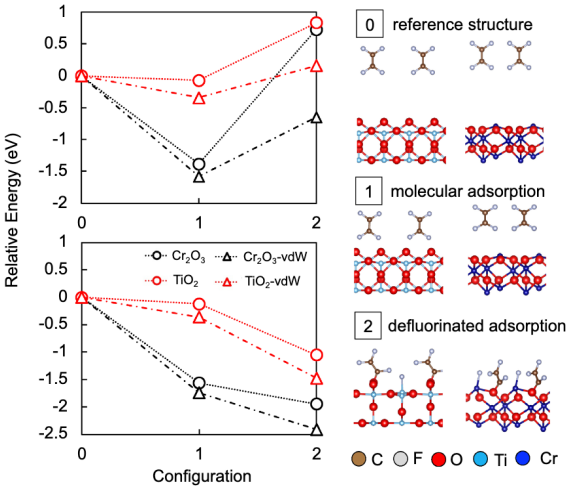

Fig. 1. (Right panel) A depiction of TFE interaction with TiO_2(110) and Cr_2O_3(0001) in 3 different configurations, viz., reference structure (0), molecular adsorption (1), and defluorinated adsorption (2) on the corresponding surfaces. Upper left panel shows the corresponding relative energies for optimized adsorbates on frozen surfaces. Lower left panel shows the corresponding relative energies upon surface relaxation. (Note stronger TFE adsorption on Cr_2O_3(0001) than on TiO_2(110). Energy trends remain even after implementing van der Waals (vdW) correction). (Taken from [5]).

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