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

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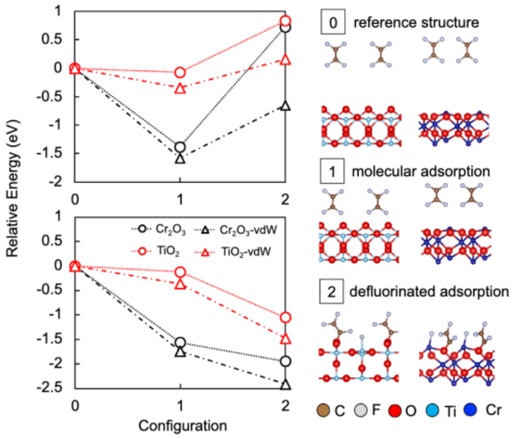
Abstract

Being able to join dissimilar materials allows design engineers to create new structures or parts with tailor-engineered properties, e.g., exhibiting high temperature resistance in one area and good corrosion resistance in another. Notable examples include polymer-metal composites used in various specialized applications. All these applications fundamentally start with polymer adhesion on metal surfaces. We showed that metal oxide surfaces catalyze the formation of intermediate defuorinated tetrafuoroethylene (TFE) radicals, resulting in enhanced binding on the corresponding metal oxide surfaces (cf., Figure: 1). 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.

Figure: 1: (Right panel) A depiction of TFE interaction with TiO2(110) and Cr2O3(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 Cr2O3(0001) than on TiO2(110). Energy trends remain even after implementing van der Waals (vdW) correction). (Taken from [1]).



Recent Publications

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3. *Y. Tsuda et al., Sci. Rep. 11 (2021) 3906-1-8.*
4. *J.S. Gueriba et al., e-J. Surf. Sci. Nanotech. 18 (2020) 307-311.*
5. *Y. Hikita et al., Optik 224 (2020) 165529-1-7.*

Biography

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1999: Doctor of Engineering, Osaka University.
1999-2001: Japan Society for the Promotion of Science (JSPS) Special Invited Foreign Researcher Fellow.
2001-2002: The University of Tokyo, Institute Industrial Science Researcher.
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