Supplementary material (ESI) for Journal of Materials Chemistry

Theoretical Study of the Surface Modification of Indium Tin Oxide with Trifluorophenyl Phosphonic Acid Molecules: Impact of Coverage Density and Binding Geometry

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SUPPLEMENTARY INFORMATION:

Adsorption Geometries of Phosphonic Acid Molecules on ITO

at Coverage Density *n*=2

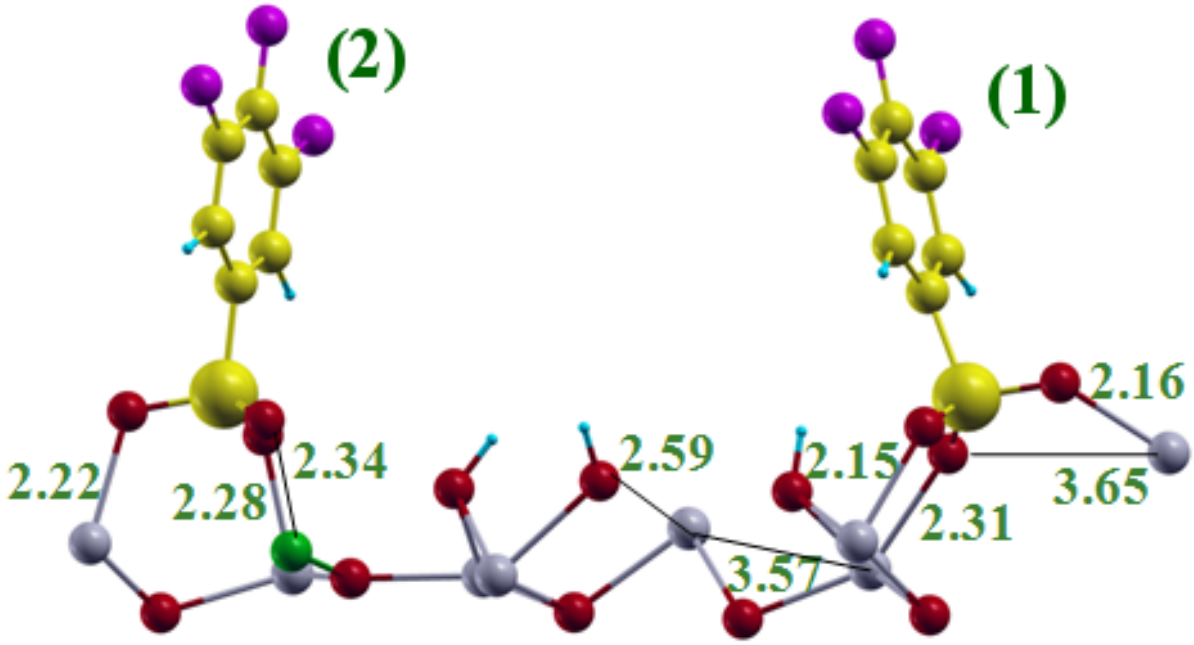

Figure S1. Side view of the fully optimized adsorption geometry of two PA molecules at site-1 and site-2. Only part of the ITO surface is shown. The values in green represent optimized bond lengths (in Å).

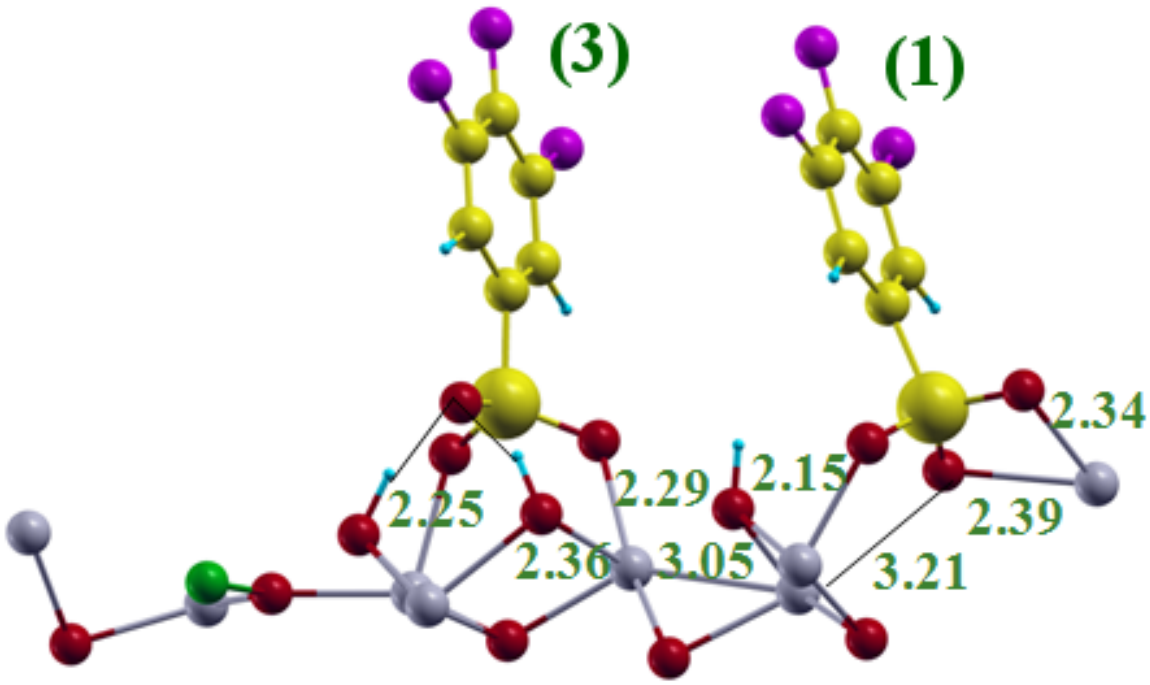

Figure S2. Side view of the fully optimized adsorption geometry of two PA molecules at site-1 and site-3. Only part of the ITO surface is shown. The values in green represent optimized bond lengths (in Å).