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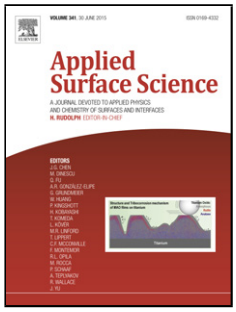

Title: The adsorptions of fixed groups −CN, $-NH_2$, −SH, −OH and −COOH of dye molecules on stoichiometric, oxygen vacancy and Pt-doped SnO_2 (110) surfaces

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ACCEPTED MANUSCRIPT

The adsorptions of fixed groups -CN, -NH_2, -SH, -OH and -COOH of dye molecules on stoichiometric, oxygen vacancy and Pt-doped SnO_2 (110) surfaces

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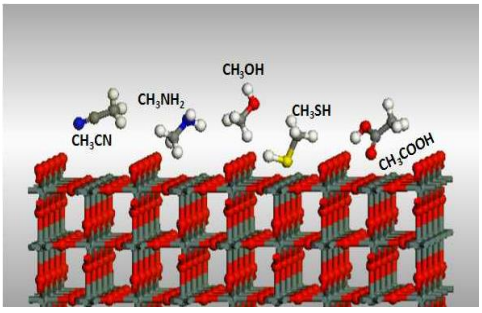
Graphical Abstract

The adsorption of CH_3CN, CH_3NH_2, CH_3SH, CH_3OH and CH_3COOH on SnO_2 (110) surface.



Highlights

- ・The adsorptions of fixed groups -COOH, - OH, -CN, -NH_2 and -SH of dye molecules on three kinds of SnO_2 (110) surfaces were systematically investigated by first principles calculations.
- ・-COOH group shows excellent adsorption performance and the Pt-doped SnO_2（110）surface is the most stable surface for the fixed groups.

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