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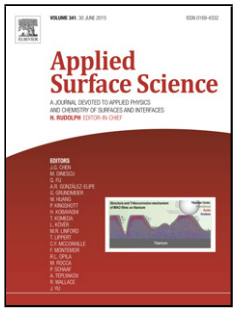

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Effects of single metal atom (Pt, Pd, Rh and Ru) adsorption on the photocatalytic properties of anatase TiO_2

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Highlights

- Due to charge transfer from metal atoms to anatase TiO_2 (101) surface, the work function of adsorbed surface is significantly smaller than the clean one, indicating enhanced surface activity.
- Fukui functions are highly localized around the isolated metal atoms (Pt, Pd, Rh and Ru), indicating that single metal atoms on anatase TiO_2 serve as the active reduction and oxidation sites in the photocatalytic process.
- Due to the metal atoms adsorption, the upward shift of conduction band edge will improve the reducing capacity of anatase TiO_2.
- When single metal atoms are adsorbed, potential energy of topmost surface Ti atoms turns to get close to the vacuum level, facilitating the electron transfer for hydrogen evolution.

Abstract

The effects of single metal atom (Pt, Pd, Rh and Ru) adsorption on the photocatalytic properties of anatase TiO_2 are investigated by means of the first-principles calculations based on density functional theory (DFT). Our results show that the most stable adsorption site for single metal atom on anatase TiO_2 (101) surface is the bridge site formed by two twofold coordinated oxygen (O_{2c}) atoms at the step edge. Due to the charge transfer from metal atoms to anatase TiO_2 (101) surface, the work function of adsorbed surface is significantly smaller than the clean one, indicating enhanced surface activity. Fukui functions are highly localized around the isolated metal atoms,

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