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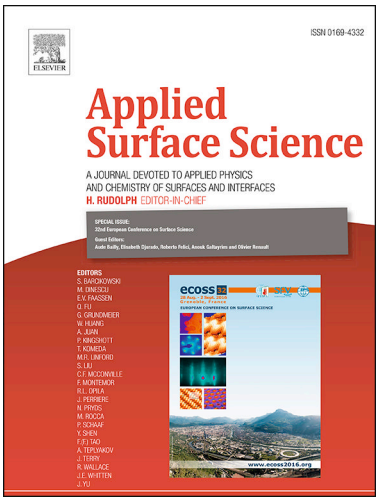

Full Length Article

The role of electric field in enhancing separation of gas molecules (H_2S, CO_2, H_2O) on VIB modified g-C_3N_4 (001)

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The role of electric field in enhancing separation of gas molecules (H_2S, CO_2, H_2O) on VIB modified g-C_3N_4 (001)

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Abstract: In this study, the first-principles calculations were performed to investigate the adsorption behaviors of gas molecules H_2S, CO_2 and H_2O on Cr, Mo and W modified g-C_3N_4 (001) surface. The results show that H_2S, CO_2 and H_2O are physically adsorbed on the pristine g-C_3N_4, while the adsorption becomes chemisorbed due to the introduction of transition metals which significantly improve the interfacial electron transfer and narrow the band gap of g-C_3N_4 (001). Furthermore, it is found that the adsorption behaviors can be greatly influenced by the applied electric field. The adsorption energy is generally arranged in the order of $E_{ads}(H_2S) > E_{ads}(H_2O) > E_{ads}(CO_2)$, and W/g-$C_3N_4$ (001) exhibits the best separation capability. The study could provide a versatile approach to selectively capture and separate the mixed gases in the catalytic reactions by controlling the applied intensity of electric field.

Keywords: g-C_3N_4 (001); electric field; molecular adsorption; first-principles calculations