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The role of electric field in enhancing separation of gas molecules

(H₂S, CO₂, H₂O) on VIB modified g-C₃N₄ (001)

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Abstract: In this study, the first-principles calculations were performed to investigate the adsorption behaviors of gas molecules H₂S, CO₂ and H₂O on Cr, Mo and W modified g-C₃N₄ (001) surface. The results show that H₂S, CO₂ and H₂O are physically adsorbed on the pristine g-C₃N₄, 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-C₃N₄ (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 $E_{\text{ads}}(\text{H}_2\text{S}) > E_{\text{ads}}(\text{H}_2\text{O}) > E_{\text{ads}}(\text{CO}_2)$, and W/g-C₃N₄ (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-C₃N₄ (001); electric field; molecular adsorption; first-principles calculations

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