Metal-doped C_3N monolayer for H_2O, CO_2, C_2H_4, and C6-aldehyde Adsorption: A DFT Investigation

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Developing gas sensors for modern agriculture is crucial for detecting molecules and chemical signals in plants that indicate plant stress, negatively impacting their growth.[1,2] Nowadays, two-dimensional materials are increasing due to their high surface-to-volume ratio, which enhances gas adsorption, and their tunable electronic properties that can improve sensing performance in gas-sensing devices.[3] In this study, we utilized density functional theory (DFT) to investigate the adsorption and gas-sensing mechanisms of C_3N monolayers for gases (H_2O, CO_2, C_2H_4, and C6-aldehyde) on both pristine C_3N and C_3N doped with metals (Al, Mg, and Na). The results showed that all metal atoms strongly bonded to the C_3N surface, with Al-doped C_3N showing the highest interaction with CO_2, C_2H_4, and C6-aldehyde molecules gas. Mg-doped C_3N demonstrated moderate interactions, particularly with H_2O molecules. Conversely, Na-doped C_3N showed the weakest interactions. Bader charge analysis indicated that molecules gas act as electron donors or acceptors from the C_3N surface, except in the case of Na-doped C_3N, where molecules gas act as electron donors. The recovery time calculations demonstrated that metal doping significantly improved the gas-sensing performance compared to pristine C_3N, particularly for H_2O, CO_2, and C_2H_4 in the Al-doped C_3N system. Our study proposes an effective strategy to enhance the adsorption and gas-sensing mechanisms of C_3N and the gas-sensing properties of C_3N, making it suitable for modern agricultural applications where detecting plant stress-related gases is essential for monitoring crop health and growth.

References

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