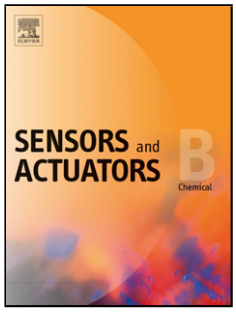

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C_3N monolayers as promising candidates for NO_2 sensors

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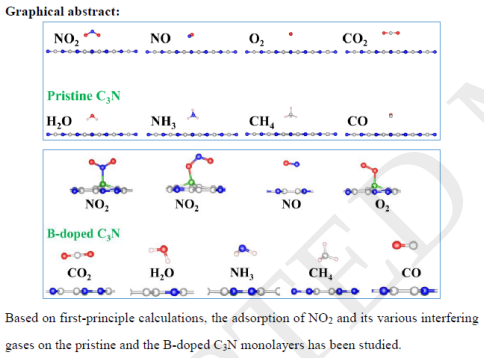
Graphical abstract



Based on first-principle calculations, the adsorption of NO_2 and its various interfering gases on the pristine and the B-doped C_3N monolayers has been studied.

Highlights

- 1, The adsorption of NO_2 and its various interfering gases on the C_3N monolayer has been theoretically studied.
- 2, The pristine C_3N monolayer is predicted to be a good room-temperature NO_2 sensor.
- 3, The doping of B atoms into the C_3N lattice is highly thermodynamically favorable.
- 4, The doped B should can further enhance the sensing selectivity and sensitivity of the C_3N monolayer toward NO_2.