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C₃N monolayers as promising candidates for NO₂ sensors

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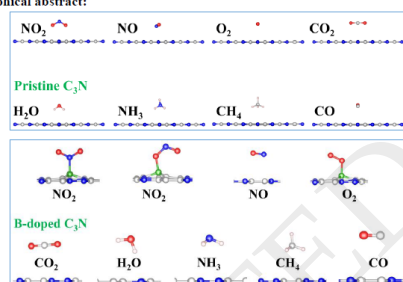
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Graphical abstract

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Based on first-principle calculations, the adsorption of NO₂ and its various interfering gases on the pristine and the B-doped C₃N monolayers has been studied.

Highlights

- 1, The adsorption of NO₂ and its various interfering gases on the C₃N monolayer has been theoretically studied.
- 2, The pristine C₃N monolayer is predicted to be a good room-temperature NO₂ sensor.
- 3, The doping of B atoms into the C₃N lattice is highly thermodynamically favorable.
- 4, The doped B should can further enhance the sensing selectivity and sensitivity of the C₃N monolayer toward NO₂.

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