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Full Length Article

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## **ACCEPTED MANUSCRIPT**

# Enhanced Carbon Monoxide Sensing Properties of $TiO_2$ with Exposed (001) facet: A Combined First-principle and Experimental Study

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### Highlight

- Anatase TiO<sub>2</sub> nano-polyhedron with highly reactive (001) facet was successfully synthesized
- First-principle calculation were carried out to expound the sensing mechanism
- (001)-dominated sensor exhibit superior response at various CO concentrations

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