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Promoting mechanism of N-doped single-walled carbon nanotubes for O₂ dissociation and SO₂ oxidation

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Highlights

- Both the N-doping pattern and the curvature of SWCNTs play key roles in tuning their catalytic performance.
- For graphite N-doped SWCNTs, the barrier for O₂ dissociation decreases with the decrease of the curvature or with the increase of the doping number of N atoms.
- The most effective catalyst for O₂ dissociation and subsequent SO₂ oxidation is dual graphite N doped (8, 8)_{out}, with an overall barrier 0.62 eV.

Abstract

Although heteroatom doping in carbon based catalysts have recently received intensive attentions, the role of the intrinsically porous structure of practical carbon materials and their

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