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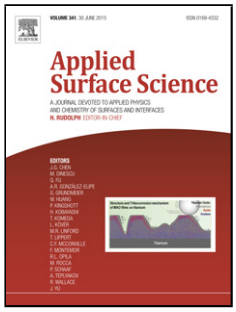

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Authors: Yanqiu Chen, Shi Yin, Yang Chen, Wanglai Cen, Jianjun Li, Huaqiang Yin

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Promoting mechanism of N-doped single-walled carbon nanotubes for O_2 dissociation and SO_2 oxidation

Yanqiu Chen[1], Shi Yin[2]*, Yang Chen[3], Wanglai Cen[1]*, Jianjun Li[2], Huaqiang Yin[2]

1. Institute of New Energy and Low Carbon Technology, Sichuan University, Chengdu 610065, P. R. China;

2. College of Architecture and Environment, Sichuan University, Chengdu 610065, P. R. China.

3. Guangxi Zhuang Autonomous Region Environmental Monitoring Center, Nanning 530028, P. R. China

Corresponding Author:

Shi Yin (yinshi_scu@foxmail.com)

Wanglai Cen (cenwanglai@163.com)

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 O_2 dissociation decreases with the decrease of the curvature or with the increase of the doping number of N atoms.
- The most effective catalyst for O_2 dissociation and subsequent SO_2 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