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Title: First-principles study of structural and work function properties for nitrogen-doped single-walled carbon nanotubes

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Highlights

- **Substitutional nitrogen atom doping in capped (5, 5) SWNT is investigated.**
- Serious defects **appear** from **breaks of C–N bonds** with N **contents of above** 23.3 at.%.
- Work function drops after N doping and may reach 4.1 eV.

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