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O₂ dissociation on nitrogen doped carbon nanotubes (10, 0) from first principles simulation SHIZHONG YANG, Southern University/LONI Institute, GUANG-LIN ZHAO, EBRAHIM KHOSRAVI, Southern University — Reducing the amount of precious platinum (Pt) loading by identifying non-precious metal catalyst is essential for large-scale applications of fuel cells, which provide a cleaning energy technology. Recent experimental, theoretical, and simulation works accelerate the advance in the research area of doped carbon nanotubes acting as an alternate non-precious metal catalyst for dioxygen reduction in the fuel cells. First principles spin polarized density functional theory(DFT) simulations have been performed to understand O₂ dissociation on nitrogen doped carbon nanotubes. We have studied nitrogen substitutional doping of carbon nanotubes (CNTs) for dioxygen adsorption, reduction, and dissociation. The calculated results show that nitrogen prefers to stay at the open-edge of short CNTs. Two O₂ chemisorption sites are found, the carbon-nitrogen complex (Pauling site) and carbon-carbon long bridge (long bridge) sites. The spin polarized DFT calculations using the nudged elastic band (NEB) method show that O₂ dissociation at the Pauling site has a reaction energy barrier of about 0.55 eV. The unique open-edge structure and charge redistribution are crucial to the novel properties of nitrogen-doped CNTs as a new non-precious metal catalyst for fuel cells.

Shizhong Yang
Southern University/LONI Institute

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