**Oxygen Vacancy Enhanced Gas Sensing Performance of CeO₂/Graphene Heterostructure at Room Temperature**

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Abstract

Oxygen vacancies (O v) as the active sites have significant influences on the enhanced gas sensing performance of metal oxide. In this paper, hydrothermal process is adopted to fabricate the composites of graphene and CeO₂ nanoparticles, in which H₂O₂ (L(+)-ascorbic acid (AA)) as the oxidant (reducing agent) is adopted to reduce (increase) the concentration of Ce³⁺ ions. It is found that the sensitivity of the composites to NO₂ is increased gradually, as the concentration of Ce³⁺ is increased from 14.6% to 50.7%, but decreases if the concentration of Ce³⁺ is higher than 50.7%. First-principles calculations illustrates that CeO₂ becomes metallic at the Ce³⁺ concentration of < 50.7%, the chemical potential of electrons on surface decreases and the fermi level shifts upwards, resulting in reduced Schottky barrier height (SBH) at the CeO₂/Graphene interface, enhanced interfacial charge transfer and high gas sensing performance. However, deep energy level is induced at the Ce³⁺ concentration of > 50.7%, and CeO₂ behaves as a semiconductor, the fermi level is pinned at the interface. As a result, the density of free electrons is reduced, leading to increased SBH and poor gas sensing response.

References