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Absorption of Carbon Monoxide Molecules On Carbon Nanotubes[1] LIANGBO LIANG, VINCENT MEUNIER, Rensselaer Polytechnic Institute — Carbon nanotubes (CNTs) have been demonstrated to be promising nanoscale molecular sensors for detecting gas molecules such as NH3, NO2 and O2. But pristine CNTs show limitations in detection of highly toxic gases such as carbon monoxide (CO). In our work, interaction of CO molecules with both armchair and zigzag single-walled CNTs (SWCNTs) has been investigated through Density Functional Theory (DFT) simulations using the software VASP. SWCNTs with structural deformation, Stones-Wales (SW) defects or single vacancy (SV) defects are considered. It has been found that structural deformation, resulting in the significant change of local physical properties, enables strong chemical absorption of CO molecules on the surface of CNTs. In addition, a SV defect also brings about dramatic change in the local geometrical structure and higher chemical reactivity, facilitating strong binding of one and two CO molecules on CNTs. Compared to pristine and SW-defect CNTs, deformed and SV-defect CNTs are more promising as gas sensors to detect toxic carbon monoxide molecules.

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Liangbo Liang
Rensselaer Polytechnic Institute

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