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Probing the Stability of Nickel Titanium Surfaces for Oxygen Adsorption: A DFT Study

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NiTi-based intermetallic compounds are known as shape memory materials and are frequently utilized in industries like aerospace, machinery, medical applications, and electronics. This is due to their structure memory effect, super elastic behaviour, high tensile strength, and biocompatibility. However, this NiTi alloy is still a contentious material due to its unstable surface and oxidation during use, more importantly, their restricted surface characteristics and adsorption process. Density functional theory (DFT) was employed in this study to investigate the surface stability and oxygen adsorption on NiTi (1 1 0) and (1 0 0) surfaces. Surface energies were analysed and it was found that the NiTi (1 1 0) surface with the lowest surface energy value is more stable than the (1 0 0) surface. In addition, oxygen adsorption was carried out on NiTi (1 1 0) surface at different adsorption sites such as the apex, bridge and hollow sites to determine the oxidation mechanism. It was found that oxygen adsorption at three possible adsorption sites and their reaction occurs spontaneously, which is attributed to the negative adsorption energy values. More importantly, the bridge site of NiTi (1 1 0) is considered the most favourable, as it has stable adsorption energy compared to other surface sites. The findings will have a good impact on the understanding of the surface stability and oxidation mechanism of NiTi surfaces.
Keywords: NiTi alloys, adsorption, surface energy, DFT

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

Hons

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