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Computational study of TiNbVZrX (X= Hf, Cr) refractory high entropy alloys

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High entropy alloys (HEAs) are a new class of materials that exhibit promising structural and functional properties, particularly in the field of hydrogen storage. However, the materials and methods used for hydrogen storage currently pose challenges, resulting in the limited storage capacity. Refractory elements are identified as potential candidates for developing effective materials for hydrogen storage. To enhance our understanding of refractory HEAs, the structural and mechanical properties of these alloys were investigated using density functional theory (DFT). The results indicate that both alloys primarily adopt a body-centered cubic (BCC) configuration. TiNbVZrHf and TiNbVZrCr alloys demonstrate excellent stability and mechanical strength, making them promising candidates for hydrogen storage and high-temperature applications. Furthermore, the alloys were found to have high thermal stability which is crucial for long-term hydrogen storage solutions. These findings highlight the potential of refractory HEAs in advancing hydrogen storage technologies.

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Primary author: Ms MOTSONONE, Lebogang (University of Limpopo)

Co-authors: Prof. CHAUKE, Hasani (University of Limpopo); Prof. NGOEPE, Phuti (University of Limpopo); Dr DIALE, Ramogohlo (Mintek)

Presenter: Ms MOTSONONE, Lebogang (University of Limpopo)

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