

Showcasing a work exploring the passivating surface oxide layers on TiFe hydrogen storage material from a group of researchers within a collaborative effort between Helmholtz Zentrum Hereon and Lawrence Livermore National Laboratory.

Influence of near-surface oxide layers on TiFe hydrogenation: mechanistic insights and implications for hydrogen storage applications

A fundamental understanding of the air-exposed TiFe surface and its interaction with hydrogen is provided in this article, along with an in-depth computational exploration of the nature and composition of the surface oxide layers. Energetics of hydrogen migration through oxide layers, motifs for the appearing oxide phases with SOAP similarities, and mechanistic insights for activation of the material are reported.



