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High density H₂ associative absorption on Titanium alpha-borozone (Ti₂B₆H₆): An ab-initio case study¹ ALIREZA AKBARZADEH², C.J. TYMZCAK³, Texas Southern University — Hydrogen is considered as a clean energy carrier that could be a future replacement for our addiction to fossil fuels. However, in order to have hydrogen economy at its highest efficiently we need to store hydrogen at high volumetric and gravimetric density. Using the all electron hybrid density functional theory, we have designed a benzene-like-molecule, Ti₂B₆H₆, which has the promise of achieving this goal. Our results show that the molecule can associatively absorb the hydrogen up to ten percent by weight of hydrogen, which exceeds the 2015 US department of energy target. In this presentation we will discuss the mechanisms of H₂ absorption and possible applications of this novel molecule.

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