

Abstract Submitted
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Transition Metal-Ethylene Complexes as High-Capacity Hydrogen Storage Media E. DURGUN, S. CIRACI, Physics Department, Bilkent University, Ankara Turkey, W. ZHOU, TANER YILDIRIM, NIST Center for Neutron Research and University of Pennsylvania — From first-principles calculations, we predict that a single ethylene molecule can form a stable complex with two transition metals (TM) such as Ti. The resulting TM-ethylene complex then absorbs up to ten hydrogen molecules, reaching to gravimetric storage capacity of 14 wt%. Dimerization, polymerizations and incorporation of the TM-ethylene complexes in nanoporous carbon materials have been also discussed. Our results are quite remarkable and open a new approach to high-capacity hydrogen storage materials discovery.

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