Abstract Submitted
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Thermodynamics of MgH_2 hydrogen storage materials: nanoparticle size and topological structure effects[1] JASON REICH, Chemisry, University of Illinois, Urbana-Champaign, IL 61801, LINLIN WANG, DUANE JOHNSON, Ames Laboratory/US DoE, Iowa State University, Ames, IA 50011-3020 — Via plane-wave-based Density Functional Theory calculations, we investigate H-desorption from (110) rutile MgH_2, a surface step, and surfaces of nanoscale $Mg_{30}XH_{62}$ clusters having catalytic dopants (X=Mg, Ti, or Fe). All calculated desorption enthalpies are endothermic, in contrast to results in the literature,[2] and no particle size effect is found for desorption of H singly, doubly, or triply-bonded to metal atoms, indicating only local bond energy is relevant. In contrast to recent results, we show that exothermic results are not obtained when initial cluster structures are carefully relaxed globally via simulated annealing, in which amorphous structures are found to be favored. A topological feature is identified that offers potential utility for using nanostructured MgH_2 as a hydrogen-storage solution.

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[2]Larsson, P.; Araujo, C. M.; Larsson, J. A.; Jena, P.; Ahuja, R. *P Natl Acad Sci USA* 2008, 105, 8227

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