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Mass Transport in the Dehydrogenation Reaction of $\mathbf{B_{20}H_{16}}$ KYLE MICHEL, CHRISTOPHER WOLVERTON, Northwestern University — The compound $B_{20}H_{16}$ has been predicted to decompose directly into 20B and $8H_2$ with favorable hydrogen release (6.9 wt. %) and equilibrium temperature ($T = 20$ °C at a pressure of 1 bar H_2) [W.Q. Sun, et. al. Phys. Rev. B. **83**, 064112, 2011]. The segregation of B and H during this reaction is investigated using density functional theory assuming that this process is mediated by the diffusion of native point defects in solid $B_{20}H_{16}$. Using the calculated formation energies under relevant chemical conditions, those defects that form in the largest concentrations, and thus those that facilitate mass segregation, are identified. These results are used to gain insight into the possible kinetic limitations of this hydrogen storage reaction.

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