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Kinetic Analysis of Gas Splitting on Oxide Surfaces for Solar Thermochemical Fuel Production[1] HEINE HANSEN, BRYCE MEREDIG, CHRIS WOLVERTON, Northwestern University, Department of Materials Science and Engineering — Solar thermochemical cycles have the potential to convert solar energy into chemical fuels at high thermodynamic efficiency. This can be done by reducing an oxide at high temperature and oxidizing the reduced oxide at a lower temperature in H_2O or CO_2 to produce H_2 or CO. The gas splitting reaction at low temperature is kinetically limited, possibly from slow kinetics of the surface processes. For example, the rate of H_2O splitting over CeO_2 is increased by the addition of a rhodium catalyst. Little is known about the gas splitting reactions at the atomic level. In this work we use density functional theory to investigate the mechanism for the gas splitting reactions on oxide surfaces such as $CeO_2(111)$ or on precious metal catalyst particles such as Rh or Pt.

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