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First-principles study of $MnNiO_3$ as an alkaline oxygen-evolution photocatalyst JIE YU, Joint Center for Artificial Photosynthesis, Lawrence Berkeley National Laboratory, QIMIN YAN, Molecular Foundry, Lawrence Berkeley National Laboratory, WEI CHEN, ANUBHAV JAIN, Environmental Energy Technologies Division, Lawrence Berkeley National Laboratory, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory, KRISTIN PERSSON, Environmental Energy Technologies Division, Lawrence Berkeley National Laboratory — We present a first-principles study of $MnNiO_3$, a promising oxygen-evolution photocatalyst. Using density functional theory with the screened hybrid functional of Heyd, Scuseria, and Ernzerhof (HSE), we compute and analyze the ground-state geometry and electronic structure. We find that $MnNiO_3$ is a ferrimagnetic semiconductor with an indirect band gap, consistent with experimental observations. We also predict that $MnNiO_3$ has promising band edge positions relative to the vacuum, with potential to straddle the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) redox potentials in aqueous solution. A detailed analysis of the band structure and density of states provides a clear explanation why $MnNiO_3$ is promising for OER. Pourbaix diagram calculations suggest that $MnNiO_3$ is stable in alkaline solution at potentials relevant for oxygen evolution. This work was supported by the Department of Energy through the Joint Center for Artificial Photosynthesis.

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