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Ternary cobalt spinel oxides for solar driven hydrogen production: Theory and experiment ARON WALSH, KWANG-SOON AHN, SUDHAKAR SHET, MUHAMMAD N. HUDA, TODD DEUTSCH, HELI WANG, JOHN A. TURNER, YANFA YAN, MOWAFAK M. AL-JASSIM, SU-HUAI WEI, National Renewable Energy Laboratory — Discovery of a chemically stable, light absorbing and conductive metal oxide with band edges aligned to water redox potentials has been a goal of physical scientists for the past forty years. Despite an immense amount of effort, no solution has been uncovered. We will present the results of our combined theoretical and experimental exploration of a series of unconventional ternary cobalt spinel oxides, which offer chemical functionality through substitution on the tetrahedral spinel A site. First-principles predictions of the substitution of group 13 cations (Al, Ga, In) in Co_3O_4 to form a series of homologous CoX_2O_4 spinel compounds are combined with experimental synthesis and photoelectrochemical characterization. Ultimately, while tunable band gaps in the visible range can be obtained, the material performance is limited by poor carrier transport properties associated with small polarons. Future design pathways for metal oxide exploration will be briefly discussed.

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