Photocatalysts for water splitting that are active under visible light have the potential to provide a sustainable supply of hydrogen for energy generation and storage. Many oxide photocatalysts have band gaps too large for the visible light region of the solar spectrum. Replacing some oxide anions with sulfide anions, forming oxysulfides, can decrease the band gap towards the visible region.[1] In addition to the band gap and band edge positions, other design features may enhance electron-hole separation and photocatalytic performance, including the cation electron configuration, polar coordination environments and a polar crystal structure.[2] The structural chemistry of oxysulfides, in terms of dimensionality and homoleptic vs heteroleptic coordination environments is not yet fully understood[3] but is thought to be critical to optimising photocatalytic activity.[4]

Our research focuses on quaternary oxysulfides. We combine experiment and theory to design and prepare new phases, and to investigate the roles polarity and connectivity, coordination environment and cation electron configuration. We present here work on La2O2MS2-related materials (Fig. 1).

Density functional theory calculations have been used to investigate the electronic structure of synthetic targets, and formation energy calculations have helped choose between synthesis routes including traditional high-temperature solid-state reactions, ball-milling methods and topotactic reactions.[5, 6]

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