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Determination of crystal structure and the study of electronic properties of $AgBiW_2O_8$ by density functional theory[1] PRANAB SARKER, MUHAMMAD N. HUDA, Physics Department, University of Texas at Arlington, Texas 76019 — $AgBiW_2O_8$ shows promising features in solar energy to hydrogen conversion through photoelectrochemical (PEC) approach because of moderate band gap, stability in the liquid solution, suitable band edge positions and low production cost. However, there is not much study available to determine its crystal structure. Using mineral database of relevant oxides and density functional theory (DFT) total energy calculation, we have determined the crystal structures of $AgBiW_2O_8$ to be a wolframite structure, which contradicts a previous report. Our theoretical electronic structure and optical properties calculation agrees well with the recent experimental result.

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