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The absolute energy positions of conduction and valence bands of selected semiconducting minerals

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ABSTRACT

The absolute energy positions of conduction and valence band edges were compiled for about 50 each semiconducting metal oxide and metal sulfide minerals. The relationships between energy levels at mineral semiconductor-electrolyte interfaces and the activities of these minerals as a catalyst or photocatalyst in aqueous redox reactions are reviewed. The compilation of band edge energies is based on experimental flatband potential data and complementary empirical calculations from electronegativities of constituent elements. Whereas most metal oxide semiconductors have valence band edges 1 to 3 eV below the H₂O oxidation potential (relative to absolute vacuum scale), energies for conduction band edges are close to, or lower than, the H₂O reduction potential. These oxide minerals are strong photo-oxidation catalysts in aqueous solutions, but are limited in their reducing power. Non-transition metal sulfides generally have higher conduction and valence band edge energies than metal oxides; therefore, valence band holes in non-transition metal sulfides are less oxidizing, but conduction band electrons are exceedingly reducing. Most transition-metal sulfides, however, are characterized by small band gaps (<1 eV) and band edges situated within or close to the H₂O stability potentials. Hence, both the oxidizing power of the valence band holes and the reducing power of the conduction band electrons are lower than those of non-transition metal sulfides.