

**Isostructural FeS<sub>2</sub> and RuS<sub>2</sub> in Solar Cells as  
Water Oxidation Photocatalysts and as  
Energy Source for Bacterial Oxidation**

Helmut Tributsch<sup>1</sup>

<sup>1</sup>Hahn-Meitner-Institut  
Dept. Solare Energetik  
Glienicker Str. 100  
Berlin 14109  
Germany

The semiconducting materials FeS<sub>2</sub> and RuS<sub>2</sub> with their identical crystalline (pyrite) structure and analogous electronic structure exhibiting d-valence bands offer the unique opportunity to learn about interfacial photoelectrochemical reactivity in context with significant challenges in energy conversion. Both materials have shown to yield high quantum efficiencies, but RuS<sub>2</sub> photooxidizes water to molecular oxygen (in a potential assistant reaction) while FeS<sub>2</sub> reacts with water to yield iron sulfate. It thereby dissolves while the RuS<sub>2</sub> interface remains stable. Metal sulfide oxidizing bacteria like *Thiobacillus ferrooxidans* or *Leptospyrilum ferrooxidans* readily oxidize FeS<sub>2</sub> to extract chemical energy while they are unable to attack RuS<sub>2</sub>. All-electrons-first-principle-calculations demonstrated a strong correlation between near band gap electronic states and the sulfur pair bond length. Iron oxidation within the FeS<sub>2</sub> interface leads to an increase of sulfur reactivity with the formation of thiosulfate. Oxidation of ruthenium within the RuS<sub>2</sub> interface, in contrast, maintains a low sulfur reactivity with the consequence that the ruthenium water complex is further oxidized until oxygen evolves. The reasons for the different behavior are analyzed and possible conclusions discussed for the design of model systems for photoelectrochemical energy conversion and photocatalysis.