Exploring Highly Active Photocatalysts at Extreme Conditions

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The obtainment of a photocatalyst with high activity and stability remains a great challenge for harvesting sunlight as storable clean fuels. A pressing need is to explore a novel method to tune the electronic band sturctures and insight into the structure-property relationships [1], [2]. In our study, the high pressure and temperature techniques are adopted to modulate the optical band gap, charge transport properties, and then photocatalytic activity of several semiconductors (Figure 1) [3]. For example, silver orthophosphate possesses a band gap of 2.4 eV. At elevated pressure, its band gap narrowed to 1.8 eV, reaching the optimal value for efficient water splitting. The band gap shrinking was related to the phase transitions and coordination number change of silver, which was illuminated by synchrotron X-ray diffraction experiments combined with the crystal structure sesearch based on the first-priciples calculations. After releasing the pressure to ambient pressure, the narrowed band gap could be partially retained.

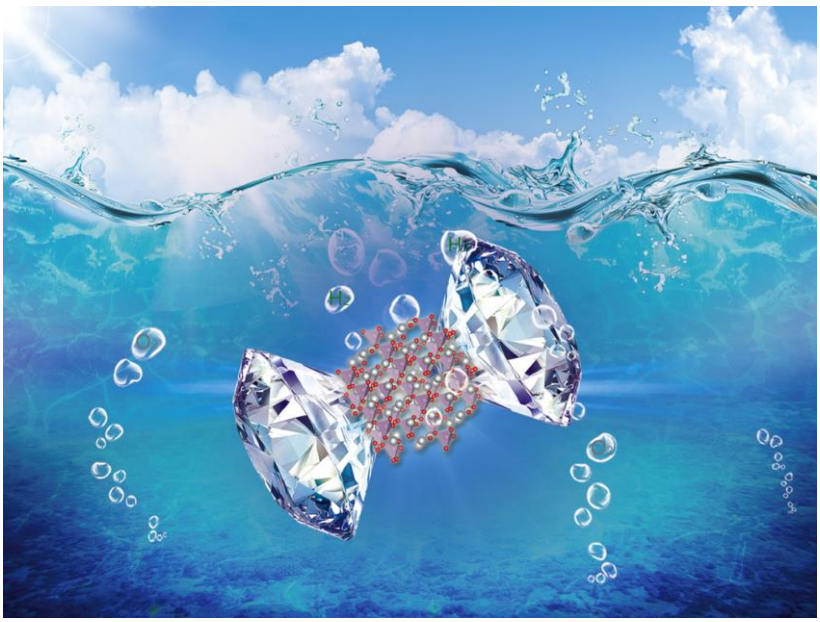

Figure 1. Photocatalytic water splitting at extreme conditions.

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