Shape effects on stability of Cu_2O particles in water and photocatalytic water splitting reaction

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Cuprous oxide (Cu_2O) has attracted attention because of its small bandgap energy, direct bandgap structure, its suitable band structure for water splitting, high absorption coefficient, the fact that it is non-toxic and its large abundance. However, it possesses a poor stability due to the fickle oxidation states of copper. In this work, Cu_2O particles of three different shapes were prepared with distinct surface structures: cubes, octahedra, and rhombic dodecahedra. Their shape stability was estimated in deionized water with or without light irradiation. The $Cu_2O(100)$ facets were selectively deformed under dark conditions, as expected from density functional theory calculations. The rhombic dodecahedra showed the most violent degradation under light irradiation, with many large thorns appearing on the surface. When water splitting was attempted using the shaped Cu_2O particles, the rhombic dodecahedra produced the most hydrogen, whereas the cubes produced none. A conformal $TiIrO_X$ overlayer was successfully formed on the rhombic dodecahedral Cu_2O particles, and the coated particles presented overall water splitting producing both hydrogen and oxygen. They also showed significantly improved stability over repeated water splitting reactions relative to bare Cu_2O particles.