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Microfaceting of Cu_2O and its implications in photochemistry YUNJAE LEE, TAEHUN LEE, YONGHYUK LEE, ALOYSIUS SOON, Department of Materials Science and Engineering, Yonsei University — The high Miller-index microfacets e.g. {211}, {311}, and {522} have been proposed to play a key role in shape-controlled crystal engineering of Cu_2O polyhedrons for various clean energy applications. These Cu_2O microcrystals with high Miller-index microfacets are found to have a higher photocatalytic activity than those with octahedra and cube morphologies, and thus suggesting that the catalytically active sites are more abundant on the high Miller-index surfaces. Although much effort has been devoted to the actual synthesis and characterizations of these shaped Cu_2O nanocrystals with various morphologies, a firm theoretical understanding of these system are currently limited to low Miller-index facets of Cu_2O. Here, we perform first-principles density-functional theory (DFT) calculations to study the surface energetics and electronic structure of these high Miller-index Cu_2O surfaces, and evaluate their overpotential for water redox reactions on Cu_2O, in comparison with that for the low Miller-index surfaces.

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