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Promote Water Photosplitting via Tuning Quantum Well States in Supported Metal Clusters ZIJING DING, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, ZI LI, GANG LU, Department of Physics and Astronomy, California State University, Northridge, California 91330-8268, USA, SHENG MENG, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — In an effort to facilitate water photosplitting at surfaces, we identify quantum well states of magic gold clusters supported on ultrathin MgO/Ag(001) as the key to favor sunlight absorption and photocatalytic reactions. Based on density functional theory (DFT) and time-dependent DFT calculati ons, the adsorption geometry, electronic structures, and excited state properties of supported metal nanoparticles can be precisely controlled. By decreasing the thickness of MgO film, charge transfer to supported gold clusters, and therefore the occupation and energy spacings of quantum well states, can be gradually tuned, leading to redshifted and enhanced plasmonic excitations and optimized energy levels for water splitting. Using nudged elastic band (NEB) and constrain DFT, we further calculate the barriers for water splitting in the ground state as well as in excited states. The barriers are found correlated with adsorption sites of water on the gold cluster. Surface hopping calculations indicate the lifetime of excited states is long enough to induce water photo-dissociation.

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