Abstract Submitted
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**Enhanced photocatalytic $H_2$ production by sub-nanometer Au nanoparticles** SHEN ZHAO, Department of Materials Science and Engineering, Stony Brook University, YAN LI, Computational Science Center, Brookhaven National Laboratory, PEICHUAN SHEN, Department of Materials Science and Engineering, Stony Brook University, DONG SU, Center for Functional Nanomaterials, Brookhaven National Laboratory, ALEXANDER ORLOV, Department of Materials Science and Engineering, Stony Brook University — CdS surfaces were found to exhibit a dramatically enhanced photo-catalytic activity for the water splitting process when loaded with sub-nanometer Au particles, compared to that of bare CdS or CdS modified with other noble metal particles (Pt, Ru, Rh, Pd) with similar co-catalyst loading. As a first step towards understanding the striking photocatalytic activity of Au/CdS, we conducted a detailed characterization of the Au particle samples by combining mass spectroscopy, (scanning) transmission electron microscopy, UV-vis spectroscopy and first-principle calculations. In particular, we carried out systematic studies of the influence of particle size, surface termination and charge state on the structural, electronic and spectroscopic properties of ligand-protected Au nanoparticles using density functional theory and time-dependent density functional theory. The structural and electronic stability of diphosphine-protected $Au_9$ and $Au_{11}$ cations with composition determined from mass spectroscopy, were confirmed from total energy and electronic structure calculations, while the computed optical absorption spectra were found to be in excellent agreement with UV-vis data. Work is underway to study the interaction between Au particles and Cds.

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