

Abstract Submitted  
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**Role of Pt nanoparticles in photocatalytic activities of CdS surfaces: Atomic and Electronic structure of Pt/CdS interface** SEFA DAG, LIN-WANG WANG, Lawrence Berkeley National Laboratory — CdS photocatalyst is one of the important material for solar cell applications and it has a profound interest in academical and industrial area. By using first-principles Density Functional theory method, we analyzed the physical characteristics behind the the outstanding catalytic activity of the Pt/CdS heterostructures. We found strong bonding interaction in the interface region between Pt and CdS and this interaction promotes new surface states occur in the band gap. Our calculations also reveal that interface dipole at the Pt/CdS interface was created by this bonding interaction and differ with respect to number of Pt layers.

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