

Abstract Submitted
for the PSF15 Meeting of
The American Physical Society

First-Principles Study of Photocatalytic Activation of CO₂ on Graphene-Semiconductor Heterostructures¹ HAIYING HE, STEPHEN SEKOULOPOULOS, STAN ZYGMUNT, Valparaiso University — The effective capture and conversion of solar energy is of critical importance for sustainable energy development. Photocatalysts are a key component in harnessing solar energy and facilitating chemical reactions to produce high-energy content chemicals. It has been reported recently that by adding graphene to semiconductor nanostructures to form composites, their photocatalytic activities can be significantly enhanced. In this work, we investigate the adsorption and initial activation of CO₂ on free-standing ZnO nanoclusters, and ZnO nanoclusters supported on graphene using the first-principles approach. A variety of binding configurations of CO₂ on different binding sites on ZnO and the activation of CO₂ will be presented and the effect of the substrate graphene will be discussed.

¹The funding support from the Indiana Space Grant Consortium (INSGC) is gratefully acknowledged.

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Date submitted: 16 Oct 2015

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