First-Principles Study of Photocatalytic Activation of CO\textsubscript{2} on Graphene-Semiconductor Heterostructures\textsuperscript{1} 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 CO\textsubscript{2} on free-standing ZnO nanoclusters, and ZnO nanoclusters supported on graphene using the first-principles approach. A variety of binding configurations of CO\textsubscript{2} on different binding sites on ZnO and the activation of CO\textsubscript{2} will be presented and the effect of the substrate graphene will be discussed.

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Haiying He
Valparaiso University

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