Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

First-Principles Study of Single Atom Catalyzed Photoelectrochemical Reduction of CO_2[1] HAIYING HE, YESUKHEI JAGVARAL, Department of Physics and Astronomy, Valparaiso University — Production of synthetic chemical fuels from solar energy is critical for us to meet the globally growing need of energy as the fossil fuels are depleting fast. The greenhouse gas CO_2, as the major product of consumption of both fossil fuels and solar fuels, can be used as the feedstock for solar fuels, thereby providing a sustainable way of closing the carbon cycle. The conversion rate of CO_2 to fuels is, however, still too low to be practical besides the poor selectivity of products. In this study, we have investigated the use of single metal atoms supported on graphene sheets as catalysts for the photoelectrochemical reduction of CO_2 using the first-principles approach. Reaction pathways to produce a variety of products such as CO, HCOOH, HCHO, CH_3OH and CH_4 will be presented to demonstrate the differences in metals with a focus on their efficiency and selectivity. Potential candidates of better catalytic performance for production of fuels are identified through computational screening.

[1]Funding support from the Indiana Space Grant Consortium (INSGC) is gratefully acknowledged.

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Date submitted: 07 Nov 2016 Electronic form version 1.4