Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

First-principles calculations of Fischer-Tropsch processes catalyzed by nitrogenase enzymes[1] JOEL VARLEY, LARS GRABOW[2], JENS NØRSKOV[3], Stanford University — The nitrogenase enzyme system of the bacteria *Azotobactervinelandii*, which is used in nature to catalyze ammonia synthesis, has been found recently to catalyze the efficient conversion of carbon monoxide (CO) into hydrocarbons under ambient temperature and pressure [1]. These findings indicate that nitrogenase enzymes could inspire more efficient catalysts for electrochemical CO and CO_2 reduction to liquid fuels. The nitrogenase variants, in which vanadium substitutes the molybdenum in the active site of the enzyme, show distinct features in their reaction pathways to hydrocarbon production. To compare and contrast the catalytic properties of these nitrogenase enzymes, we perform first-principles calculations to map out the reaction pathways for both nitrogen fixation and for the reduction of CO to higher-order hydrocarbons. We discuss the trends and differences between the two enzymes and detail the relevant chemical species and rate-limiting steps involved in the reactions. By utilizing this information, we predict the electrochemical conditions necessary for the catalytic reduction of CO into fuels by the nitrogenase active sites, analogous to a Fischer-Tropsch process requiring less extreme conditions.

[1] Y. Hu, C.C. Lee, M.W. Ribbe, Science **333**, 753 (2011)

[1] This work was supported by the Global Climate and Energy Project (GCEP) at Stanford University.

[2] University of Houston

[3] SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory

Joel Varley
Stanford University

Date submitted: 02 Dec 2011
Electronic form version 1.4