

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Catalytic role of defective carbon in the methane decomposition for CO and CO₂-free hydrogen generation LIPING HUANG, Department of Chemical and Biomolecular Engineering, North Carolina State University; Department of Physics, North Carolina State University, ERIK SANTISO, Department of Chemical and Biomolecular Engineering, North Carolina State University, MARCO BUONGIORNO NARDELLI, Department of Physics, North Carolina State University; CSMD, Oak Ridge National Laboratory, KEITH GUBBINS, Department of Chemical and Biomolecular Engineering, North Carolina State University — Decomposition of methane is an environmentally attractive approach to CO and CO₂-free hydrogen production. The decomposition of methane over defective carbon was studied by using state of the art first principles modeling techniques. Our studies demonstrate that the defective carbon itself can be used as catalyst for methane decomposition, without the need for other catalysts like transition metals or oxides, and the catalytic sites in defective carbon can be regenerated by the deposition of carbon decomposed from methane, to make the hydrogen production a continuous process. Additionally; since no other gases are produced in the process, the cost of CO₂ sequestration and hydrogen purification from CO contamination will be dramatically reduced.

Liping Huang
Department of Chemical and Biomolecular Engineering,
Department of Physics; North Carolina State University

Date submitted: 02 Dec 2006

Electronic form version 1.4