Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Stabilization mechanisms of polar ZnO surfaces revisited SHENGBAI ZHANG, National Renewable Energy Laboratory, MAO-HUA DU, STEVEN ERWIN, Naval Research Laboratory, JOHN NORTHRUP, Palo Alto Research Center — The polar (0001) surfaces of ZnO exhibit a variety of different morphologies. The mechanisms underlying this diversity have not been definitively identified. Here we evaluate the role of several possible candidates. We show that electrostatics does not play a significant role. Instead, we argue that surface morphology is determined by a competition between two other mechanisms. The first is the electron counting rule, which leads to semiconducting surfaces. The second arises from the large cohesive energy of ionic crystals such as ZnO, which tends to preserve the surface stoichiometry at its bulk value, leading to metallic surfaces. First-principles calculations show a crossover in the relative stability of semiconducting and metallic surfaces as the chemical potential of oxygen is varied. This behavior accounts for the many observed surface morphologies on ZnO(0001), including triangular islands and pits.

Shengbai Zhang
National Renewable Energy Laboratory

Date submitted: 20 Nov 2006 Electronic form version 1.4