Generalized Electron Counting in Determination of Metal-Induced Reconstruction of Compound Semiconductor Surfaces LIXIN ZHANG, National Renewable Energy Laboratory, Golden, CO 80401, ENGE WANG, QIKUN XUE, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China, SHENGBAI ZHANG, National Renewable Energy Laboratory, Golden, CO 80401, ZHENYU ZHANG, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — Based on theoretical analysis, first-principles calculations, and experimental observations, we establish a generic guiding principle, embodied in generalized electron counting (GEC), that governs the surface reconstruction of compound semiconductors induced by different metal adsorbates. Within the GEC model, the adsorbates serve as an electron bath, donating or accepting the right number of electrons as the host surface chooses a specific reconstruction that obeys the classic electron counting model. The predictive power of the GEC model is illustrated for a wide range of elements from alkali to transition metals, and to noble metals.

Lixin Zhang
National Renewable Energy Laboratory, Golden, CO 80401

Electronic form version 1.4