Abstract Submitted for the MAR06 Meeting of The American Physical Society

Zintl Concepts for Interface Engineering ALEX DEMKOV, The University of Texas at Austin — Crystalline epitaxial oxides on semiconductors (COS) could very well extend the Complimentary Metal Oxide Semiconductor (CMOS) technology from Si to other semiconductors and thus give new lease on life to the paradigm responsible for the outstanding success of the semiconductor electronics. Another tantalizing possibility is the growth of functional oxide structures utilizing ferroelectricity, superconductivity, magnetism, and other such properties not normally accessible in conventional semiconductors in monolithic integration with Si. There also may be applications of COS at the end of the Si Roadmap. Two dimensional (2D) crystal growth of ionic oxides on covalent semiconductors and visa versa is essential for these approach to work. In this talk I will discuss how concepts developed by Edward Zintl more than seventy years ago can be used for interface engineering. I will use ab-initio density functional theory to demonstrate how the bonding character at the oxide/semiconductor interface is manipulated through charge transfer in the engineered intermetallic contact layer. This transition layer lowers the energy of the interface and results in 2D growth, and high quality epitaxial films.

> Alex Demkov The University of Texas at Austin

Date submitted: 29 Nov 2005 Electronic form version 1.4