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**Unified transition path and universal transition state  
for ZB to RS or WZ to RS high pressure phase transition**

MAOSHENG MIAO, WALTER R.L. LAMBRECHT, Case Western Reserve University — We show that the previously proposed transition paths for high pressure phase transitions for semiconductor from zinc blende (ZB) to rocksalt (RS) and from wurtzite (WZ) to rocksalt can be unified and can be extended to transitions from various tetrahedrally bonded polytypes to rocksalt [1]. Our first principle pseudopotential calculations with density functional and constrained relaxation methods on SiC showed that the ZB to RS transition has the lowest transition barrier. Our calculations on ZB to RS transition path for other semiconductors including II-VI, III-V and group IV semiconductors, show that the position and the geometry of the transition state, the state that correspond to the transition barrier, are universal and do not depend on the chemical components of the system [2]. We also extended the Landau phase transition model to a ZB to RS transition by using a cosine function of the atom displacement as order parameter. The model shows that the position of the transition state does not depend on the coupling between the atom displacement and the strains of the lattice, which is the key point that the transition state is independent of the chemical components. [1] M. S. Miao and Walter R. L. Lambrecht, Phys. Rev. B **68**, 092103 (2003). [2] M. S. Miao and Walter R. L. Lambrecht, Phys. Rev. Lett., accepted

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Maosheng Miao  
miaoms@cwru.edu  
Case Western Reserve University

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