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Universal transition state and transition path for the high-pressure zinc blende to rocksalt phase transition MAOSHENG MIAO, WALTER LAMBRECHT, Department of Physics, Case Western Reserve University — Although the high-pressure zinc blende (ZB) to rocksalt (RS) structural transition has been studied intensively in many experiments and theories, the understanding of the kinetics of this process, especially of its the transition state (TS), the saddle point on the transition path, is still incomplete. We studied the TS and energetics along a previously introduced low barrier orthorhombic transition path of the ZB to RS transition for several semiconductors, including II-VI and III-V compounds and group-IV elemental semiconductors using a first-principles full-potential linearized muffin-tin orbital method. The path is defined by the relative sublattice position and the lattice constants are allowed to relax in response to this chosen independent variable. We found that: 1) the location and the geometry of the TS are identical for all the semiconductors investigated; 2) the lattice constants and the scaled volume vary in a universal manner along the path for all the semiconductors; 3) the cosine function of the relative sublattice position can be used as an order parameter for expanding the energy associated with the the phase transition. A Landau like model for reconstructive phase transition with changing periodicity shows that the position of the transition state does not depend on the chemical components of the semiconductors.

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