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**Universal transition state and transition path for
the high-pressure zinc blende to rocksalt phase transition**

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Case Western Reserve University — Although the high-pressure zinc
blende (ZB) to rocksalt (RS) structural transition has been studied in-
tensively 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 semicon-
ductors 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 indepen-
dent 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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