## Automated identification of pathways and transition states in solid state transformations

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Determining transition paths in solid-phase transformations is a challenging task. Previously, we introduced an evolutionary method to identify the lowest energy path and transition state for pressure-induced structural transformations in solids. This method requires no user input and prior knowledge of possible paths [1]. The structures and energetics along the transition path were computed using first-principles density functional calculations. While the algorithm is robust, extending the method to large systems becomes computationally impractical. In this work, we propose a simplified approach to identifying suitable transition paths by imposing geometric constraints. Since the total energy of a system primarily depends on local bonding, which is directly related to local geometries, we can screen out energetically unfavorable trial structures by defining a "cost function." This allows for an efficient exploration of the potential energy landscape by optimizing comparisons among different trial structures. Additionally, global optimization is performed using a more efficient "Greedy algorithm." We applied this approach to study the mechanisms underlying the complex pressure-induced structural transformation sequence of Cs-II (FCC, 2 atoms/cell)  $\rightarrow$  Cs-III (*Cmcm*, 84 atoms/cell)  $\rightarrow$  Cs-IV (*I*4<sub>1</sub>*amd*, 4 atoms/cell). The results are in complete agreement with complementary molecular dynamics simulations.

## References

1. Yin, K., et.al., NPJ Comp. Mat., 2020, 6, 16.