Exploring the Lowest-Energy Structures of Boron Nitride

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Abstract

Understanding the atomic structures of materials is crucial in physics, chemistry, and materials science. Structural searches identify the most stable (lowest-energy) configurations of materials, which is essential since experimentally determining these structures can be time-consuming and technically challenging. Computational methods provide an efficient alternative, enabling material predictions without extensive experiments. In this work, we perform a structural search for boron nitride (BN), a compound widely used in cutting and grinding metals, high-temperature-resistant materials, and electrical insulators. Using the CALYPSO program, which employs particle swarm optimization (PSO) for global optimization, we generate approximately 900 different structures. Density functional theory (DFT) calculations are then used to evaluate their enthalpies. Our results reveal that the lowest-energy structures belong to the 216th space group, F-43m, providing valuable insights into BN's stability and potential applications.

Methods

Global optimization: Particle swarm optimization (PSO)[1] algorithm is used for searching low-energy crystal structures. The PSO is a "swarm-intelligence scheme for global optimization" inspired by natural systems (birds flocking) that has been applied to fields like engineering and chemical science. The algorithm mimics particles in a "swarm" and moves them around until the best possible placement is found for the lowest potential energy surface. We used the structure search program CALYPSO (Crystal structure AnaLYsis by Particle Swarm Optimization)[2,3] which implements the PSO method.

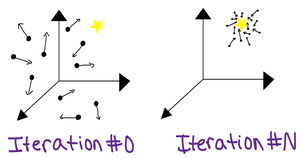

Figure 1: An illustration for the particle swarm optimization scheme.

Energy calculations: The energies of various structures are computed efficiently using the density functional theory (DFT) with an highly efficient program called VASP (Vienna ab initio simulation package). DFT is a computational quantum mechanical modeling method that calculate the total energy of a system with given atomic positions.

Results

The enthalpies of the lowest-energy structure found through the different generations of PSO are shown in Figure 2. The program ran for 30 generations, refining its search with each iteration until it identified the lowest enthalpy structure. It took the program five generations to find the lowest energy structure. Boron nitride is a relatively simple compound with a well-defined low-energy structure, making it easier for the algorithm to converge quickly. This explains why the algorithm stabilizes after the 5th generation, as further iterations yield no significant improvements. For more complex structures, we anticipate greater variation in enthalpy across generations.

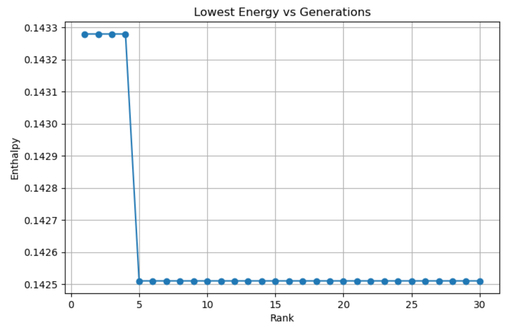

Figure 2. The evolution of the lowest enthalpy found after each PSO generations.

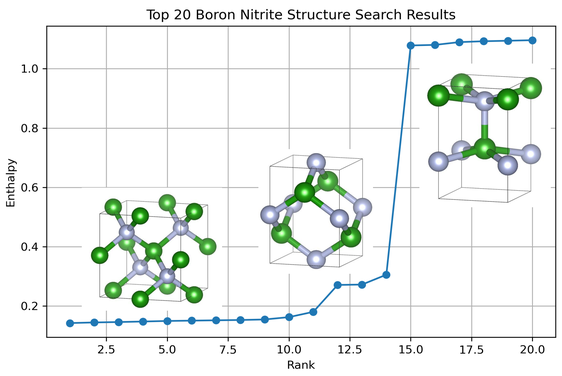

Figure 3. Ordering of 20 lowest-enthalpy structures. The first, second, and the third groups are from space group 216, 119, and 107, respectively (from left to right).

The 20 lowest-energies structures are shown in Figure 3. The space group number 216 is found to have the lowest energy structure for this compound, with space groups 119, 107, and 225 coming close behind. Each space group has a cluster of very similar structures coming from the 900 structure searches with very close enthalpies, that is why the plot remains relatively constant within each space group before transitioning to a new enthalpy minimum.

Conclusion

Through our computational structure search, we identified the lowest-energy configuration of boron nitride, corresponding to space group 216 (F-43m). Our findings highlight the efficiency of PSO-driven searches in rapidly converging on stable structures. Given the challenges of experimental synthesis and characterization, such predictive modeling provides a cost-effective and time-efficient method to identify promising material candidates. Future research will expand structure searches beyond boron nitride to explore stable configurations of other materials.

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