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Trimming a Combinatorical Tree WILEY MORGAN, ROD FORCADE, GUS HART, Brigham Young University — In computational material science, one frequently needs to know the number of unique atomic configurations in a structure. For example in an A_3B phase, two different kinds of atoms may be present on the B sites. In modeling possible alloys one needs to know the number of possible arrangements on the B sites. The obvious solution to this combinatorics problem is to generate the list of all possible configurations and then eliminate those that are symmetrically equivalent. This approach, however, suffers from a combinatoric explosion, particularly for large structures with more than two atom types. This happens even when there are a large number of symmetrically-equivalent configurations and only a few unique configurations that survive the elimination process. We developed a new algorithm that avoids this problem by not generating the entire list of configurations. Instead, it generates "partial configurations" and applies the symmetry operations without finding each "complete" configuration. This algorithm allows us to tackle much larger problems due to increases in computational efficiency.

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