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Generating and utilizing derivative structures[1]

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Derivative superstructures play an important role in different material phenomena such as chemical ordering in alloys, spin ordering in magnets, and vacancy ordering in non-stoichiometric materials. Large sets of derivative superstructures are often used in (practically) exhaustive searches of binary configurations on a lattice to determine ground state properties of intermetallic systems. Other physical observables may also be targeted if an appropriate Hamiltonian is available. We present a group-theoretic approach for generating derivative superstructures. The approach is completely general—it can be applied to any crystal type, non-Bravais lattices, mixed anion/cation double binary systems, and surface systems as well as bulk systems. We give examples of problems that can be addressed with the group-theoretic approach such as optimization of band gaps and effective masses in III-V heterostructures, significant increases of Monte Carlo cell sizes for lattice gas simulations, exhaustive testing of lattice models, and the identification of new crystal structures (and predicting the corresponding systems in which the structure may be observed).

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