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The "Inverse Band Structure (IBS) Approach" for designer nanostructures and designer impurities in semiconductors. ALEX ZUNGER, S. DUDIY, NREL — While in standard computational physics and chemistry one first defines the molecular or crystalline structure and then computes the ensuing electronic structure and properties, we adopt a reverse approach in which we search for the atomic configuration having a prescribed target property. Using either Simulated Annealing or Genetic Algorithms as search strategies we determine the configuration of groups of Nitrogen atoms having either the deepest or the shallowest level in the GaP gap, or the highest/lowest oscillator-strength for optical absorption. Similar approaches are used to determine the extremal band gaps of alloys and the configuration of Mn atoms in GaAs having the highest Curie temperature. This approach allows one to scan a large number of configurations of e.g, alloys in search of the optimal one with a desired property.If the property is readily calculable, the IBS search is done on-the-fly. If its difficult to calculate (e.g, Tc of ferromagnets), we first do a cluster expansion,then IBS search. Work supported by DOE-SC-BES-DMS under NREL contract AC3699GO10377.

Alex Zunger
NREL

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