Atomistic material design by optimization for semiconductor nanostructures

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We cast the problem of discovering atomic configurations with desired electronic structural properties as a constrained global optimization problem. Here the free variables are the location and identity of every atom in a material and the objective function is built from the desired electronic properties. For example, we can minimize the bandgap or we can optimize for a target of combined bandgap and effective mass. We present two evolutionary optimization methods (a genetic algorithm[1] and a scatter search algorithm). We present a comparison of optimization methods and direct enumeration for design of semiconductor alloys with specific electronic properties[2]. In addition, we present the optimization of electronic structural properties of branched tetrapod-shaped CdSe nanocrystals[3] for potential applications in high efficiency solar cells.

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