AlxGa1-xAs crystals with direct 2 eV band gaps from computational alchemy

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We use alchemical first order derivatives for the rapid yet robust prediction of band structures. The power of the approach is demonstrated for the design challenge of finding Al x Ga 1 − x As semiconductor alloys with large direct band gap using computational alchemy within a genetic algorithm. Dozens of crystal polymorphs are identified for x >2 3 with direct band gaps larger than 2:eV according to HSE approximated density functional theory. Based on a single generalized gradient approximated density functional theory band structure calculation of pure GaAs we observe convergence after visiting only ∼ 800 crystal candidates. The general applicability of alchemical gradients is demonstrated for band structure estimates in III-V and IV-IV crystals as well as for H 2 uptake in Sr and Ca-alanate crystals.
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