

Publication**Al_xGa_{1-x}As crystals with direct 2 eV band gaps from computational alchemy****JournalArticle (Originalarbeit in einer wissenschaftlichen Zeitschrift)****ID** 4495959**Author(s)** Chang, Kuang-Yu Samuel; von Lilienfeld, O. Anatole**Author(s) at UniBasel** [Chang, Kuang-Yu](#) ; [von Lilienfeld, Anatole](#) ;**Year** 2018**Year: comment** 2018**Title** Al_xGa_{1-x}As crystals with direct 2 eV band gaps from computational alchemy**Journal** Physical Review Materials**Volume** 2**Number** 7**Pages / Article-Number** 073802

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_xGa_{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 H₂ uptake in Sr and Ca-alanate crystals.

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