Abstract Submitted
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Finding structures with specific properties in complex configurational spaces using multi-target inverse band structure approach[1] PAULO PIQUINI, Universidade Federal de Santa Maria, 97105-900, Santa Maria, RS, Brazil, ALEX ZUNGER, National Renewable Energy Lab., Golden, CO 80401 — The conventional strategy to look for materials with desired properties is to use physical intuition to select some candidates among an enormous number of possibilities.Apart the very special cases, the solutions to these search problems are far from obvious. The inverse band structure (IBS) approach, on the other hand, search for the desired electronic structures (instead of atomic configurations) from the beginning. Here we illustrate the power of this inverse approach by applying it to the simultaneous engineering of multi-target problems, which encompass huge configurational spaces: (i) the search of a specific band gap in the quaternary (In,Ga)(As,Sb) semiconductors(a) lattice-matched to InP and, (ii) the stacking sequence of (In,Ga)As/InP superlattices leading to band gaps and strains within the range suitable for thermophotovoltaic applications(b).

(a) P. Piquini, P.A. Graf, and A. Zunger, Phys. Rev. Lett. **100**, 186403 (2008);
(b) P. Piquini and A. Zunger, Phys. Rev. B **78**, 161302 (2008)

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Paulo Piquini
UFSM

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