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Use of First-Principles Theory to Identify materials and nano structures for next-generation solar cells[1]

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Three genomic-like material design approaches are explored for finding energy relevant semiconductors: *(i) Search of nanostructure combinations leading to intermediate band solar ce*lls: Within the ideology of intermediate band solar cells (IBSC) based on quantum dots, it is presently unknown which combination of dot material + matrix material + substrate satisfies the energetic criteria enabling IBSC. Using the modern theory of nano structures (based on atomistic pseudo potentials in plane waves), we examine various combinations, finding that some of the "usual suspect" long believed to be ideal, are, in fact inappropriate. (*ii) Finding new inorganic absorbers with first-principles:* Standard compilations of inorganic compounds reveal thousands of candidate materials that were unexplored for their potential as PV absorbers, among others, because of the absence of a quantifiable "Design Principle" that sorts out various materials. The common Schockley - Queisser criteria gives a universal, gap vs efficiency curve which does not distinguish different types of gaps (direct-allowed vs direct-forbidden vs-indirect) nor does it account for non radiative recombination. A simple treatment, called "Spectroscopically Limited Maximum efficiency" (SLME) accounts for such factors and can be calculated for hundreds of compounds (using the GW approach), providing insight into previously unrecognized candidates, as well as to the mechanisms at work causing absorption enhancement.(iii) I*nverse Band structure search for direct gap Si-Ge nano structures:* Using a genomic approach to pseudo potential configurational search we identify a Si-Ge nano structures that have direct band gaps, solving the long-standing dilemma of crystalline Column IV absorbers. In collaboration with L. Yu, V. Popescu, J.W. Luo and M. Davezac.

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