Overcoming Doping Bottlenecks in wide-gap materials: What makes a TCO a TCO

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When one dopes externally an insulator or a semiconductor, at some critical position of the Fermi level (“Pinning Level”), doping is spontaneously halted .We now understand that this occurs by the self-regulating, spontaneous formation of "killer defects" .In effect, the system protects itself from the perturbing effect of doping by rearranging its bonds to minimize the perturbation,(i.e. ,a manifestation of the Le Chatellier effect).For example, when a solid is doped intentionally n-type, so the Fermi level moves towards the conduction band, at some point, cation vacancies form spontaneously. Being acceptors, they "kill" the intentionally -introduced doped electrons. Different materials differ by the position of the critical Fermi level at which this happens. In easy-to-dope materials (Si, GaAs ,InAs) this level is located inside the host bands, so doping stops only after the system is already well-doped. On the other hand, in wide gap materials needed for solid state lighting, this critical level might be inside the band gap, so doping stops before the Fermi level reaches its target position near band edges.
In this talk I will explain the ensuing physics of such self-limiting behavior, and formulate empirical rules as to how one might overcome some of these limits. I will then turn to another design problem --" impurity design”. Assuming, for the sake of discussion, that you could position impurities (such as Nitrogen in III-V's) at any relative geometry in the lattice (isolated impurities, clusters consisting of pairs or of triplets ;random impurities, etc) :which configuration will yield target physical properties ? (e.g. deepest levels; or shallowest levels; or largest oscillator strength; or minimum strain ,etc).I will describe how this Inverse Band Structure approach can be performed to the benefit of III-V nitride alloys for Solid State Lighting.