Practical doping principles

Alex Zunger

Citation: Applied Physics Letters 83, 57 (2003); doi: 10.1063/1.1584074

View online: http://dx.doi.org/10.1063/1.1584074

View Table of Contents: http://scitation.aip.org/content/aip/journal/apl/83/1?ver=pdfcov

Published by the AIP Publishing

Articles you may be interested in

First-principles theoretical analysis of transition-metal doping of ZnSe quantum dots

J. Appl. Phys. 112, 024301 (2012); 10.1063/1.4734841

Tuning the electronic and magnetic properties of carbon-doped ZnO nanosheets: First-principles prediction

J. Appl. Phys. 111, 044329 (2012); 10.1063/1.3688233

First-principles study of Be doped CuAIS 2 for p-type transparent conductive materials

J. Appl. Phys. 109

Practical doping principles

Alex Zunger^{a)}
National Renewable Energy Laboratory, Golden, Colorado 80401
(Received 27 January 2003; accepted 21 April 2003)

with killer defects, or prevent E_F from moving." An example is the use of H during Mg doping 12 of GaN: without H, excessive p-type Mg doping will lead to the spontaneous formation of V_N once the Fermi energy moves sufficiently towards the VBM. But since H acts as a donor, it prevents the movement of E_F towards the VBM, thus defeats the formation of the V_N killer defect. Subsequently, H is annealed out. This rule suggests, for example, that p-type doping of oxides can be facilitated by creating internal oxygen precipitates that eliminate oxygen vacancies, e.g., using NO or NO $_2$ sources 3,5 for nitrogen-doping of ZnO, or using Li $_2$ O sources for Li doping of MgO (Ref. 23).

(ii) Doping rules pertaining to chemical potential effects.