n-type doping $(1, 1)$ $\mathbf f$ ree holes (*p*-type doping) into the system. The paradigm

than codoping [6] ZnO by 2N Ga and is also locally stable. This principle of design of the local chemical chem bonding the verticidity ΔE_b can be used to improve the used general doping in other systems by searching for chemical additional additions by searching for chemical additions $\mathcal{L}(\mathcal{L})$ $t \mapsto \frac{1}{2}$ ΔE_{b} , which maintaining ΔH_f and shallow ionization energies.

The allowed chemical potential potential ranges of E_c (3) are decided by the host considerations. For the host $\mathbf r$ $\overline{\mathsf{O}}_{i,j}$, we have, at equilibrium

$$
+ \qquad = \Delta H_f(\quad . \quad); \tag{4}
$$

 $\mathbf{w}^{(k)} \in \Delta H_{\mathbf{f},k}$, the compound formation entries $\mathbf{h}^{(k)}$ to 2 and solid metallic \mathbf{I} and \mathbf{r} assume that the assure competing phases for elemental solids G and σ τ τ τ τ τ N2 and ² gases, and the compounds Ga2 ³, GaN, $\frac{1}{2}$ 4 *do not* f_x

$$
i \leq 0 \qquad (i = \dot{N} : \dot{N} : \dot{N} \tag{5}
$$

$$
2 + 3 \leq \Delta H_f(-_{2-3}); \tag{6}
$$

$$
+ \quad \ + \quad \ \mathbf{N} \quad \leq \Delta H_f(\quad \ \mathbf{N} \quad \) \tag{7}
$$

$$
+2+4 \leq \Delta H_f(\begin{array}{cc} 2 & 4 \end{array})
$$
 (8)

The calculated formation enthalping are -3.61 (-3.6), -11.07 (-10 *:*), and -16.24 for $\overline{0}$, $\overline{2}$ $\overline{3}$, and \widetilde{Z} a, respectively, which compare well with a value \overline{Z} able experimental values given in \mathbb{T} . The formation entry of $\mathbf{A} \mathbf{N}$ and \mathbf{A}

(iii) *n-type doping with Ga and* N_2 *source.* $F_1 \cup I(.)$ shows that using the κ is a favors ($\Delta H_f < 0$) t_1 , N_1 N_2 and N_3 N_4 N_5 N_6 which promote *n*-type *n*-type *n*-type doping, whereas the clusters $\mathrm{G}_\mathbb{N}$ $_4$ and $\mathrm{G}_\mathbb{N}$ $_3$ which $_3$ $\int_{0}^{\infty} p$ -type doping are less favorable ($\Delta H_{f} > 0$) under the these conditions. These Γ reveals that the stability that the stability of N-Ga4 results from a highly favorable bonding energy favorable bonding energy f ΔE_b

see, for example, that for S_1 cluster in S_2 cluster in \mathcal{O}_1 involves creation of 4 Ga-N and 12 Ga-O bonds and an destroying 16 Zn-O bonds. On the other hand, creating the G_N-4 cluster inside O involves making \sim 1.4 Ga-N and 12 $$ -N bonds, destroying 16 $$ -O bonds. Since $$ and $$ have three unknown excess bond energies (*E*Ga- , *E*Zn-N, and $E_{-\vec N}$) and many more calculated ΔE_b values of $(\texttt{T}_i$ is $\texttt{T}_i)$, it is straightforward to determine the excess of excess \texttt{r}_i bond energies for any doping configuration from any doping configuration from any \mathbf{f} and any simple cluster expansion 20

 $\Delta E_b(\;\; ; \;\; _F) = N^{\left(\;\; \right)} \, \frac{1}{\rm N} \; \frac{E}{\rm N} \; + N^{\left(\;\; \right)} \; \frac{E}{\rm E} \; \frac{1}{\rm C} \; + N^{\left(\;\; \right)} \, \frac{E}{\rm N} \; \frac{E}{\rm N} \; ;$ (9)

 $\mathcal{N}^{(1)}$ are the number of -