



Design of Shallow p-type dopants in ZnO

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Introduction

- ZnO is a promising material for short wave-length opto-electronic devices such as UV lasers and LEDs due to its large exciton binding energy and low material cost
- ZnO can be doped easily n-type, but the realization of stable p-type ZnO is rather difficult

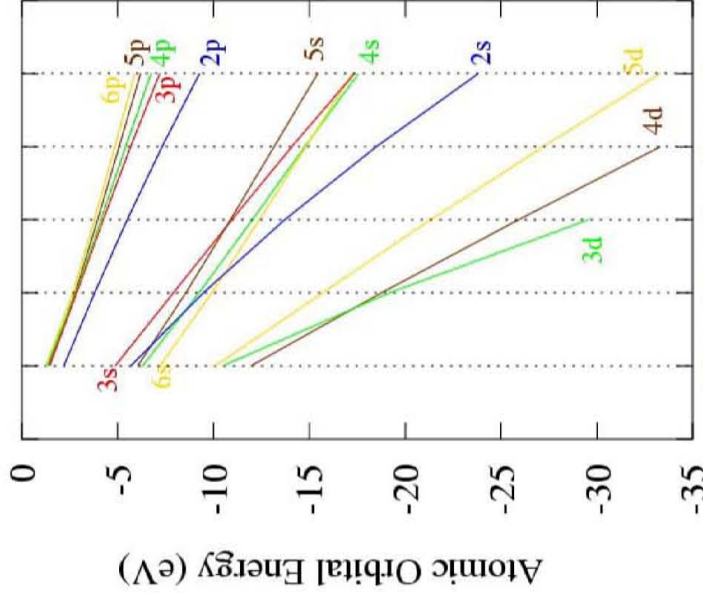
Using first-principles band structure methods we will address:

- What causes the p-type doping difficulty in ZnO
- How to overcome the p-type doping difficulty in ZnO



Chemical Trends of Atomic Energy Levels

Chemical trends of atomic energy levels



Be B C N O
Mg Al Si P S
Zn Ga Ge As Se
Cd In Sn Sb Te
Hg Tl Pb Bi Po

NIST
National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce

PERIODIC TABLE
Atomic Properties of the Elements

Group 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
IA IIA IIIA IVA VA VIA VIIA VIIIA

Period 1 2 3 4 5 6 7

Legend:
Solids (white)
Liquids (blue)
Gases (yellow)
Artificially Prepared (pink)

Frequently used fundamental physical constants:
For the most accurate values of these and other constants, visit Physics and Constants
1 second = 919,263,177 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of Cs
Speed of light in vacuum $c = 299\,792\,458\text{ m s}^{-1}$ (exact)
Planck constant $h = 6.626\,070\,15 \times 10^{-34}\text{ J s}$ (exact)
Elementary charge $e = 1.602\,176\,634 \times 10^{-19}\text{ C}$ (exact)
Proton mass $m_p = 1.672\,621\,923 \times 10^{-27}\text{ kg}$
 $\alpha = 1/137.035\,999\,074$ (exact)
Fine-structure constant
Feynman constant
Boltzmann constant
 $k_B = 1.380\,658 \times 10^{-23}\text{ J K}^{-1}$

1 ¹ H Hydrogen 1.007 84 1.007 94	2 ⁴ He Helium 4.002 602 4.002 603	3 ⁶ Li Lithium 6.941 6.940	4 ⁷ Be Beryllium 9.012 182 9.012 183	5 ⁹ B Boron 10.811 10.811	6 ¹⁰ C Carbon 12.011 12.011	7 ¹¹ N Nitrogen 14.006 43 14.006 43	8 ¹² O Oxygen 15.999 03 15.999 03	9 ¹³ F Fluorine 18.998 403 18.998 403	10 ¹⁶ S Sulfur 32.06 32.06	11 ¹⁹ K Potassium 39.098 3 39.098 3	12 ²⁰ Ca Calcium 40.078 40.078	13 ²³ V Vanadium 50.941 5 50.941 5	14 ²⁴ Cr Chromium 51.996 1 51.996 1	15 ²⁶ Fe Iron 55.845 55.845	16 ²⁷ Co Cobalt 58.933 2 58.933 2	17 ²⁸ Ni Nickel 58.693 4 58.693 4	18 ²⁹ Cu Copper 63.546 63.546	19 ³⁰ Zn Zinc 65.38 65.38	20 ³⁵ Br Bromine 79.904 79.904	21 ³⁶ Kr Krypton 83.80 83.80	22 ³⁹ Rb Rubidium 85.468 85.468	23 ⁴⁰ Zr Zirconium 91.224 91.224	24 ⁴¹ Nb Niobium 92.906 38 92.906 38	25 ⁴² Mo Molybdenum 95.94 95.94	26 ⁴³ Tc Technetium 98.906 25 98.906 25	27 ⁴⁴ Ru Ruthenium 101.07 101.07	28 ⁴⁵ Rh Rhodium 102.905 5 102.905 5	29 ⁴⁶ Pd Palladium 106.363 1 106.363 1	30 ⁴⁷ Ag Silver 107.868 2 107.868 2	31 ⁴⁸ Cd Cadmium 112.411 112.411	32 ⁴⁹ In Indium 114.818 114.818	33 ⁵⁰ Sn Tin 118.710 118.710	34 ⁵¹ Sb Antimony 121.757 121.757	35 ⁵² Te Tellurium 127.60 127.60	36 ⁵³ I Iodine 126.905 47 126.905 47	37 ⁵⁴ Xe Xenon 131.29 131.29	38 ⁵⁵ Cs Cesium 132.905 45 132.905 45	39 ⁵⁶ Ba Barium 137.327 137.327	40 ⁵⁷ La Lanthanum 138.905 138.905	41 ⁵⁸ Ce Cerium 140.12 140.12	42 ⁵⁹ Pr Praseodymium 140.907 6 140.907 6	43 ⁶⁰ Nd Neodymium 144.24 144.24	44 ⁶¹ Pm Promethium 144.912 6 144.912 6	45 ⁶² Sm Samarium 150.36 150.36	46 ⁶³ Eu Europium 151.964 151.964	47 ⁶⁴ Gd Gadolinium 157.25 157.25	48 ⁶⁵ Tb Terbium 158.925 34 158.925 34	49 ⁶⁶ Dy Dysprosium 162.50 162.50	50 ⁶⁷ Ho Holmium 164.930 32 164.930 32	51 ⁶⁸ Er Erbium 167.259 167.259	52 ⁶⁹ Tm Thulium 168.934 21 168.934 21	53 ⁷⁰ Yb Ytterbium 173.054 173.054	54 ⁷¹ Lu Lutetium 174.967 174.967	55 ⁷² Hf Hafnium 178.49 178.49	56 ⁷³ Ta Tantalum 180.947 88 180.947 88	57 ⁷⁴ W Tungsten 183.84 183.84	58 ⁷⁵ Re Rhenium 186.207 186.207	59 ⁷⁶ Os Osmium 190.23 190.23	60 ⁷⁷ Ir Iridium 192.222 192.222	61 ⁷⁸ Pt Platinum 195.084 195.084	62 ⁷⁹ Au Gold 196.966 569 196.966 569	63 ⁸⁰ Hg Mercury 200.59 200.59	64 ⁸¹ Tl Thallium 204.3833 204.3833	65 ⁸² Pb Lead 207.2 207.2	66 ⁸³ Bi Bismuth 208.980 401 208.980 401	67 ⁸⁴ Po Polonium 209 209	68 ⁸⁵ At Astatine 210 210	69 ⁸⁶ Rn Radon 222 222	70 ⁸⁷ Fr Francium 223 223	71 ⁸⁸ Ra Radium 226 226	72 ⁸⁹ Ac Actinium 227 227	73 ⁹⁰ Th Thorium 232.037 7 232.037 7	74 ⁹¹ Pa Protactinium 231.036 88 231.036 88	75 ⁹² U Uranium 238.028 91 238.028 91	76 ⁹³ Np Neptunium 237.048 17 237.048 17	77 ⁹⁴ Pu Plutonium 244.064 2 244.064 2	78 ⁹⁵ Am Americium 243.061 3 243.061 3	79 ⁹⁶ Cm Curium 247.070 35 247.070 35	80 ⁹⁷ Bk Berkelium 247.070 35 247.070 35	81 ⁹⁸ Cf Californium 251.083 3 251.083 3	82 ⁹⁹ Es Einsteinium 252.083 3 252.083 3	83 ¹⁰⁰ Fm Fermium 257.103 3 257.103 3	84 ¹⁰¹ Md Mendelevium 258.103 3 258.103 3	85 ¹⁰² No Nobelium 259.103 3 259.103 3	86 ¹⁰³ Lr Lawrencium 262.103 3 262.103 3
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Atomic Number 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300 301 302 303 304 305 306 307 308 309 310 311 312 313 314 315 316 317 318 319 320 321 322 323 324 325 326 327 328 329 330 331 332 333 334 335 336 337 338 339 340 341 342 343 344 345 346 347 348 349 350 351 352 353 354 355 356 357 358 359 360 361 362 363 364 365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 408 409 410 411 412 413 414 415 416 417 418 419 420 421 422 423 424 425 426 427 428 429 430 431 432 433 434 435 436 437 438 439 440 441 442 443 444 445 446 447 448 449 450 451 452 453 454 455 456 457 458 459 460 461 462 463 464 465 466 467 468 469 470 471 472 473 474 475 476 477 478 479 480 481 482 483 484 485 486 487 488 489 490 491 492 493 494 495 496 497 498 499 500 501 502 503 504 505 506 507 508 509 510 511 512 513 514 515 516 517 518 519 520 521 522 523 524 525 526 527 528 529 530 531 532 533 534 535 536 537 538 539 540 541 542 543 544 545 546 547 548 549 550 551 552 553 554 555 556 557 558 559 560 561 562 563 564 565 566 567 568 569 570 571 572 573 574 575 576 577 578 579 580 581 582 583 584 585 586 587 588 589 590 591 592 593 594 595 596 597 598 599 600 601 602 603 604 605 606 607 608 609 610 611 612 613 614 615 616 617 618 619 620 621 622 623 624 625 626 627 628 629 630 631 632 633 634 635 636 637 638 639 640 641 642 643 644 645 646 647 648 649 650 651 652 653 654 655 656 657 658 659 660 661 662 663 664 665 666 667 668 669 670 671 672 673 674 675 676 677 678 679 680 681 682 683 684 685 686 687 688 689 690 691 692 693 694 695 696 697 698 699 700 701 702 703 704 705 706 707 708 709 710 711 712 713 714 715 716 717 718 719 720 721 722 723 724 725 726 727 728 729 730 731 732 733 734 735 736 737 738 739 740 741 742 743 744 745 746 747 748 749 750 751 752 753 754 755 756 757 758 759 760 761 762 763 764 765 766 767 768 769 770 771 772 773 774 775 776 777 778 779 780 781 782 783 784 785 786 787 788 789 790 791 792 793 794 795 796 797 798 799 800 801 802 803 804 805 806 807 808 809 810 811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827 828 829 830 831 832 833 834 835 836 837 838 839 840 841 842 843 844 845 846 847 848 849 850 851 852 853 854 855 856 857 858 859 860 861 862 863 864 865 866 867 868 869 870 871 872 873 874 875 876 877 878 879 880 881 882 883 884 885 886 887 888 889 890 891 892 893 894 895 896 897 898 899 900 901 902 903 904 905 906 907 908 909 910 911 912 913 914 915 916 917 918 919 920 921 922 923 924 925 926 927 928 929 930 931 932 933 934 935 936 937 938 939 940 941 942 943 944 945 946 947 948 949 950 951 952 953 954 955 956 957 958 959 960 961 962 963 964 965 966 967 968 969 970 971 972 973 974 975 976 977 978 979 980 981 982 983 984 985 986 987 988 989 990 991 992 993 994 995 996 997 998 999 1000

Atomic potential becomes more negative when the atomic number increases from left to right in the Periodic Table



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Method of Calculation

Method of calculation



- Band structure and total energy are calculated using the first-principles band structure method (FLAPW, PP) with local density approximation (LDA)
- Defects are described using the supercell approach. A uniform background charge is added for charged defect calculation
- All the internal structural parameters are optimized by minimizing the quantum mechanical forces
- Band in different supercell calculations are aligned using atomic core levels or average potentials



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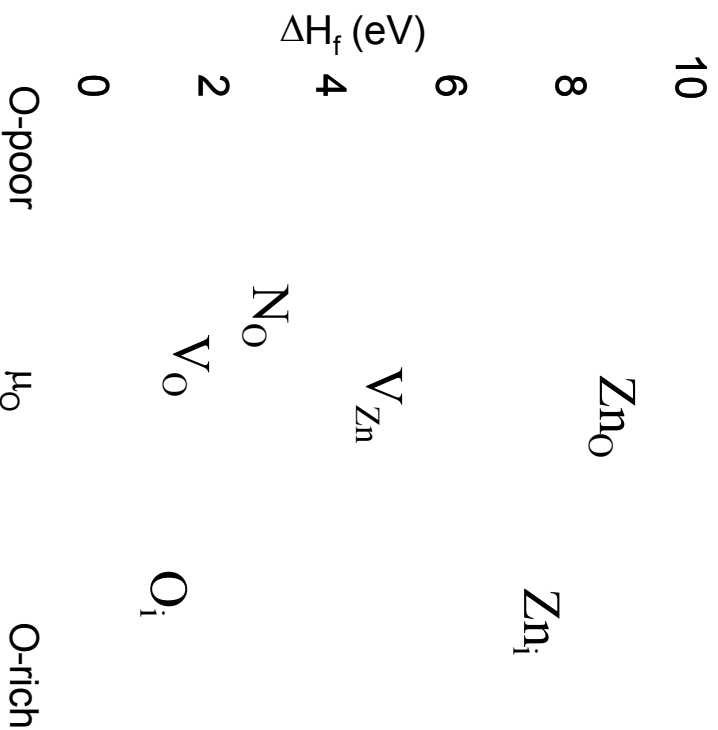
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Origin of the p-type doping difficulty in ZnO

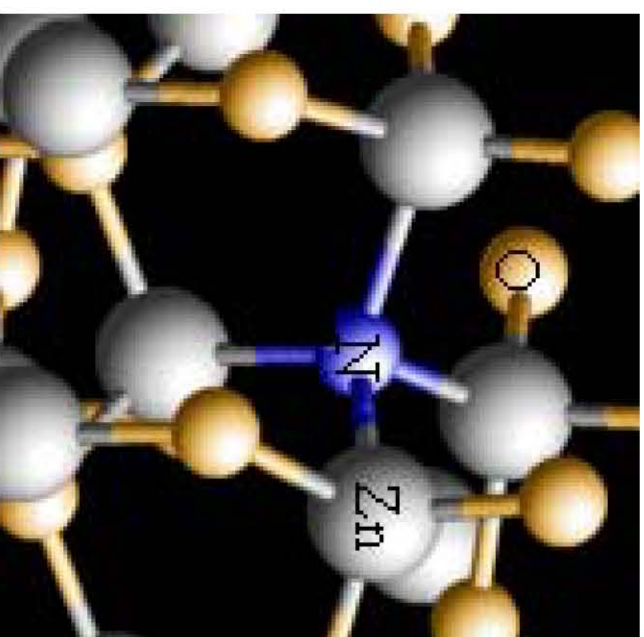
Main reasons of failure-to-dope

- The impurity atom has limited solubility in the host material, so not enough dopants are introduced
- The defect transition energy levels are too deep, so not enough charge carrier are generated at working temperature
- Spontaneous formation of opposite-charged “killer defects” (cation vacancy, anion vacancy, etc.), which pins the Fermi energy

Origin of p-type doping difficulty in ZnO: high acceptor formation energy



Due to the strong bonding and large formation energy of ZnO , intrinsic defect formation energies are large



Calculate minimum defect formation energy of neutral N_{O}

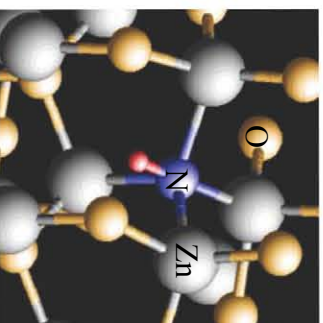
$$H_{\text{f}}(\text{N}_{\text{O}})_{\text{min}} = 1.2 \text{ eV} \quad (\text{N}_2)$$

Origin of p-type doping difficulty in ZnO: high acceptor ionization energy

Acceptor energy levels in ZnO

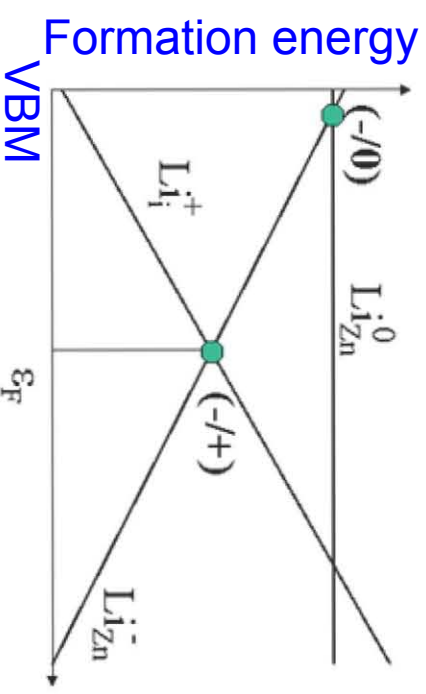
CBM

(0/-)



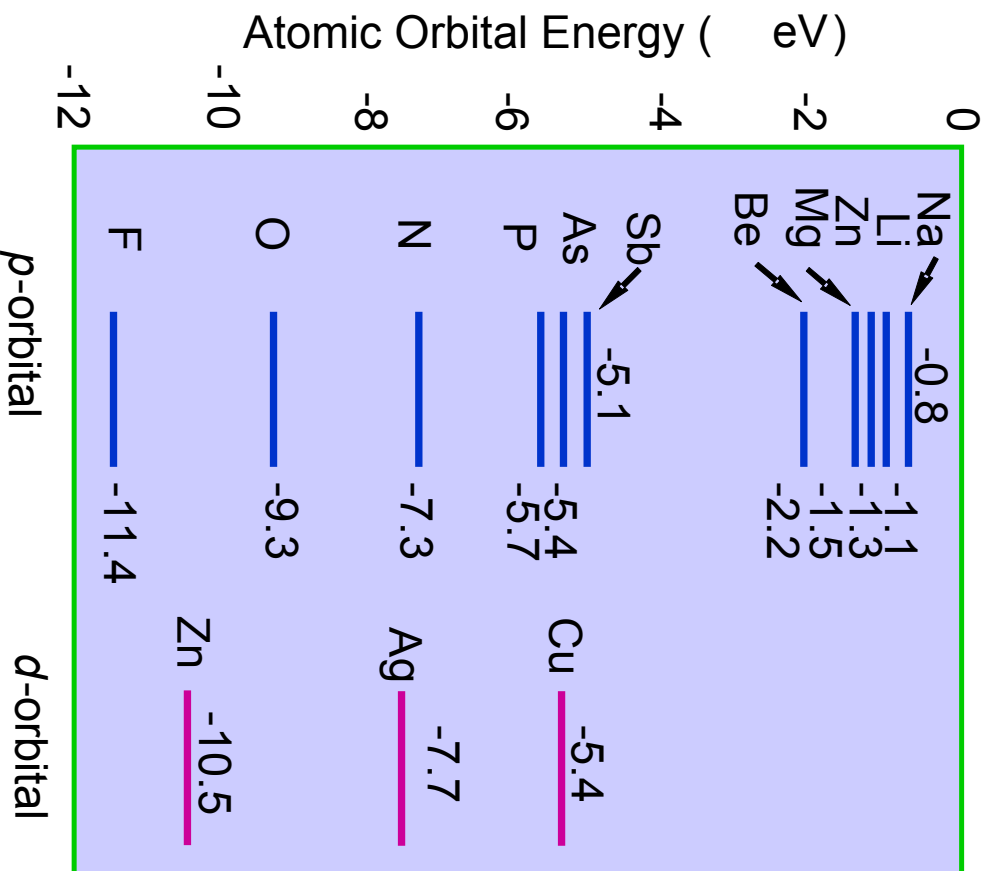
Sb _O	1.10	Cu _{Zn}	0.74
As _O	0.90	Ag _{Zn}	0.40
P _O	0.70	Na _{Zn}	0.17
N _O	0.35	Li _{Zn}	0.09
		V _{Zn}	0.34 (0/2-)
			0.18 (0/-)

VBM



- For group V on oxygen site acceptor, the lowest transition energy level N_O is 0.35 eV above the VBM
- For group IB on Zn site acceptor, the lowest transition energy level is also deep, at 0.40 eV for Ag_{Zn}
- Group IA on Zn site has relatively shallow defect level, but self compensation limits their use as effective acceptor

Origin of p-type doping difficulty in ZnO: high acceptor ionization energy



- An acceptor level above VBM has a wavefunction character similar to the VBM, i.e. it has an anion p and cation d orbital characters
- Oxygen p orbital energy is very low, there are no group-V elements that are more electronegative than O
- p - d coupling between host elements and dopants (e.g., N_O with Zn or Cu_{Zn} with O) is large



Strategies to overcome the doping limit

- Increase defect solubility by “defeating” bulk defect thermodynamics
- Reduce defect ionization level through proper codoping techniques
- Reduce defect compensation and ionization level by modifying the band edge states



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Improve the Dopant Solubility by Adjusting Dopant Chemical Potentials

Increase defect solubility using non-equilibrium thermodynamics

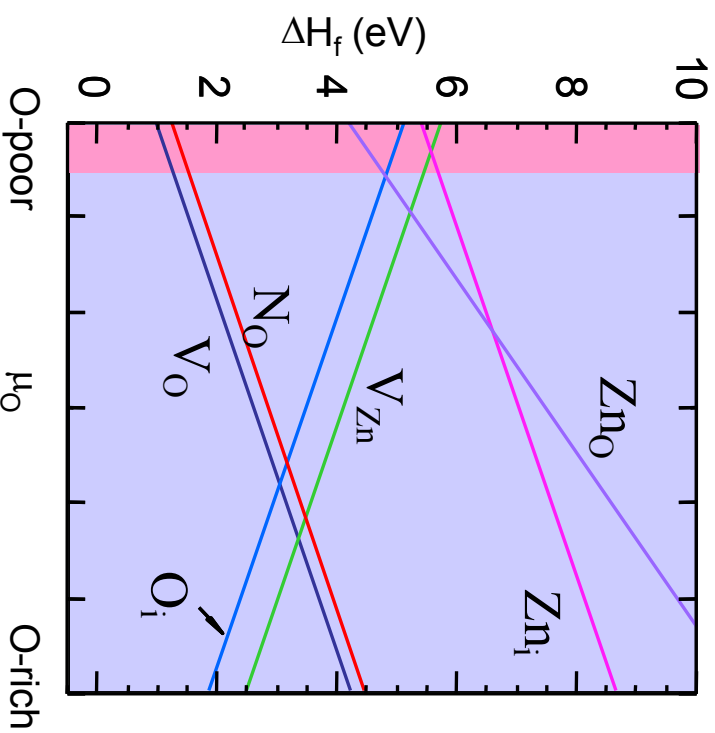
- What controls the dopant solubility is the dopant chemical potential, μ_A . Therefore, the key to enhance the solubility of the dopant is to raise the chemical potential and avoid the formation of the precipitates of the dopants

$$\Delta H^{(\alpha,q)}(E_F, \mu) = \Delta E^{(\alpha,q)}(E_F=0, \mu_i=0) + \sum n_i \mu_i + q E_F$$

- Choose the optimal host element chemical potentials
- Enhance solubility by metastable molecular doping
- Enhance solubility by epi-growth (e.g., MBE)

Choose the optimal host element chemical potentials

- The formation energy of N_O is the lowest under O-poor condition, whereas V_{Zn} is the lowest under the O-rich condition



$$\Delta H_f = E(ZnO:N) - E(ZnO) + \mu_O - \mu_N$$

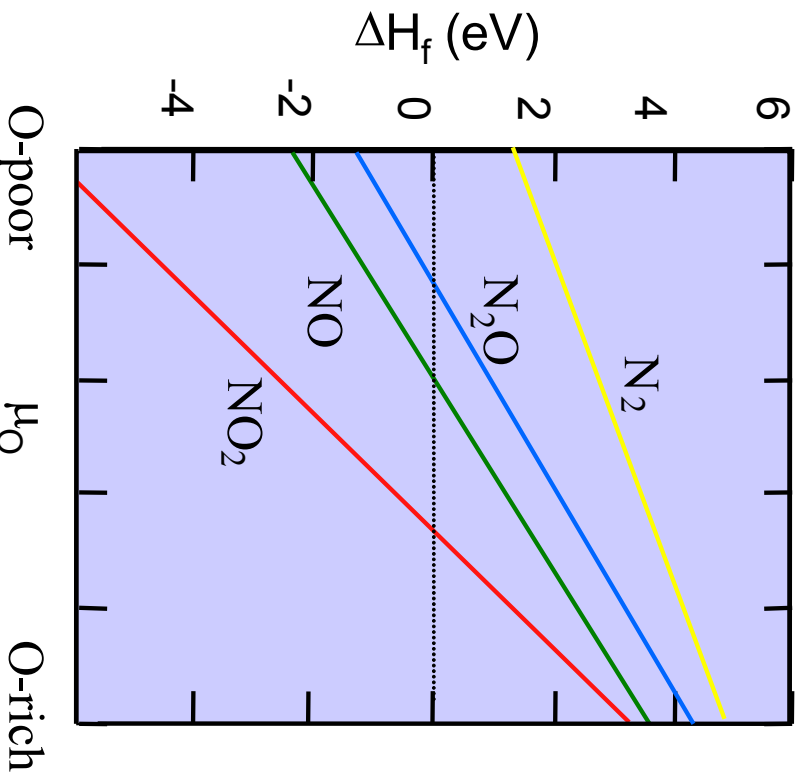
$$\Delta H_f = E(ZnO:V_{Zn}) - E(ZnO) + \mu_{Zn}$$

Enhanced solubility by molecular doping: ZnO:N

$$\Delta H_f = E(\text{ZnO:N}) - E(\text{ZnO}) + \mu_{\text{O}} - \mu_{\text{N}}$$

$$\Delta H_f = E(\text{ZnO:N}) - E(\text{ZnO}) + 2\mu_{\text{O}} - \mu_{\text{NO}}$$

$$\mu_{\text{N}}(\text{N}_2) < \mu_{\text{N}}(\text{N}_2\text{O}) < \mu_{\text{N}}(\text{NO}) < \mu_{\text{N}}(\text{NO}_2)$$

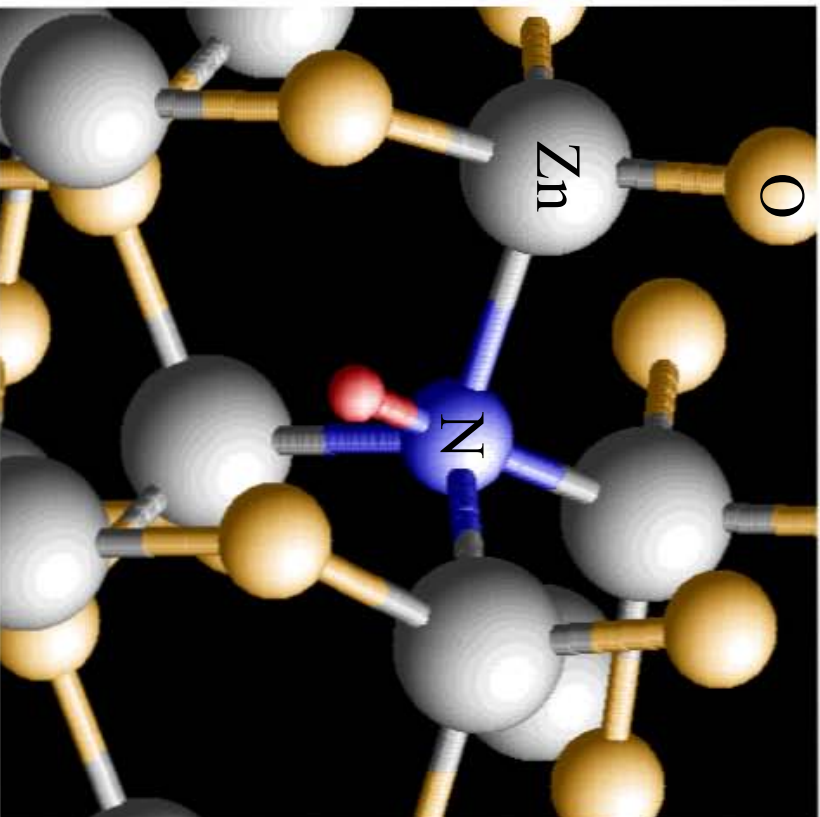


N chemical potential depends on the doping sources (N_2 , N_2O , NO , NO_2)

N solubility in ZnO is much higher if NO or NO_2 is used as dopant

NO or NO_2 doping also avoids the formation of $(\text{N}_2)_{\text{O}}$, which is a compensation donor in ZnO

Single N atom in ZnO



Transition energy level of N_o

$$E(0/-) = \text{VBM} + 0.35 \text{ eV}$$

Calculate minimum defect formation energy N_o

$$H_f(N_o)_{\min} = 1.2 \text{ eV} \quad (N_2)$$

$$H_f(N_o)_{\min} = 0.4 \text{ eV} \quad (\text{NO}, \text{Zn}_3\text{N}_2)$$



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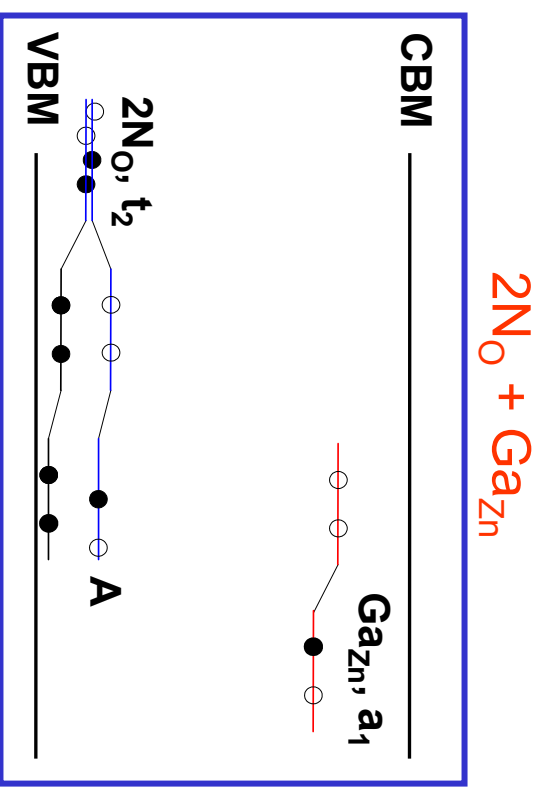
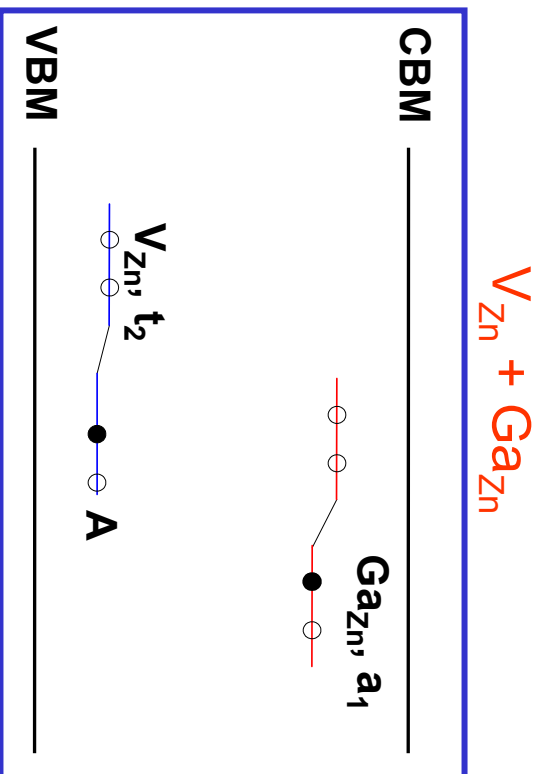
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Design shallow defect levels in ZnO using band structure calculation method

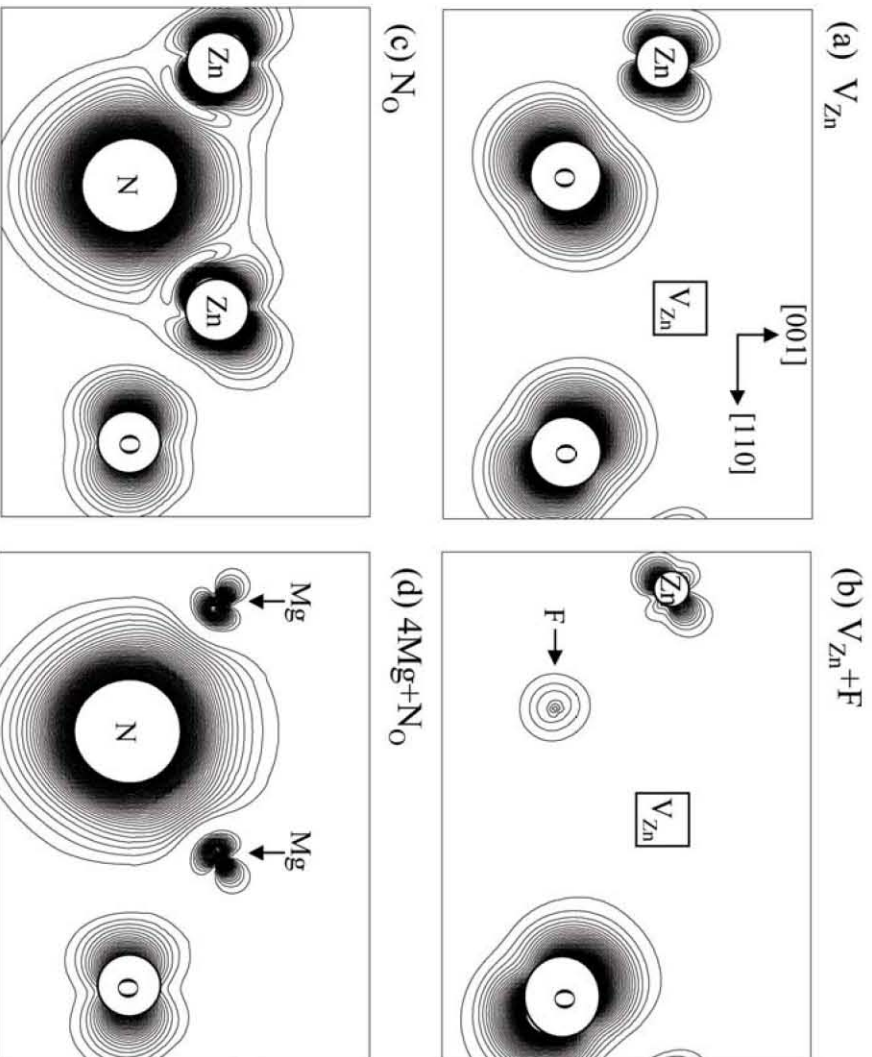
Effects of conventional co-doping

- Can co-doping lower the defect transition energy levels?



- The level repulsion effect is rather small because the donor state and the acceptor states have different symmetry
- The defect transition energy level may be lowered only if the defect complex consists a single donor and a single acceptor

Design shallow p-type dopants in ZnO



➤ Defect wavefunction has large weight on its neighboring atoms

➤ Replace O by the more electronegative F is expected to lower V_{Zn} energy level

➤ Remove p-d coupling between N_O and cation by replacing Zn with Mg or Be is also expected to reduce the acceptor energy level

$N_{O,p}$

Zn,d

A

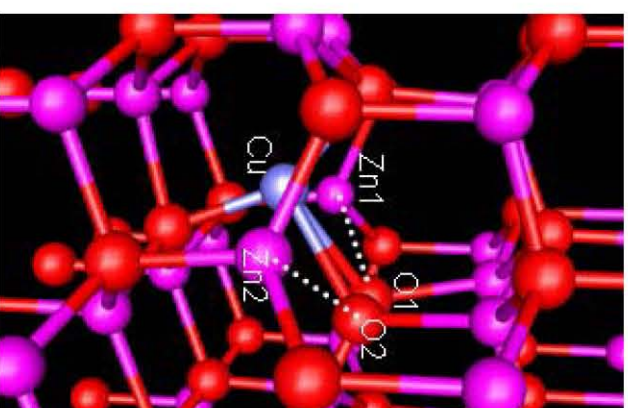
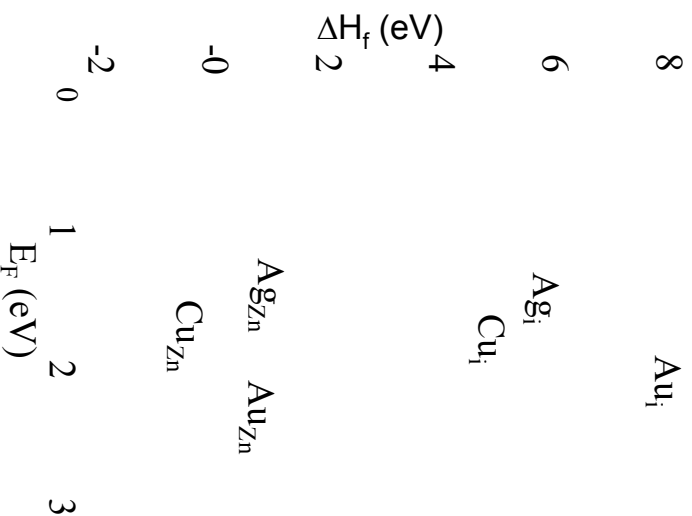
Zn,d

Design shallow p-type dopants in ZnO

Defect	E_b	(0/-)	(-/2-)
N_O		0.31	—
$N_O\text{-}MgZn$	0.3	0.29	—
$N_O\text{-}4MgZn$	1.6	0.23	—
$N_O\text{-}BeZn$	0.1	0.22	—
$N_O\text{-}4BeZn$	1.9	0.12	—
V_{Zn}		0.18	0.34
$V_{Zn}\text{-}FO$	-2.3	0.16	—

➤ The calculated defect ionization energy levels suggest that F and Be could be good p-type co-dopant for ZnO

Reduce self-compensation by introducing Group-IB acceptors in ZnO



- Cu_{Zn} has very deep acceptor level because of the large p-d coupling, but Ag_{Zn} has relatively shallower levels
- IB_i is highly unstable, so self-compensation for IB dopants is low

Large size mismatched p-type doping in ZnO:As

Background:

- p-type conductivity in As and P-doped ZnO have been observed and conventional doping model attributed the dopants to As_O and P_O
- We have show that As_O and P_O are unlikely to be the measured acceptor because
 - The formation energy is high (As and P is much larger than O)
 - The ionization energy of As_O and PO are very high ~ 0.8 eV

Acceptor energy levels in ZnO

CBM

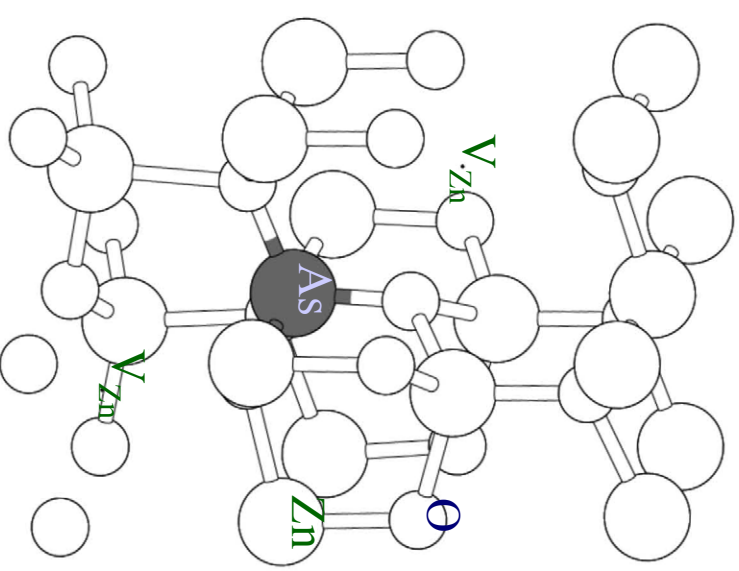
Sb_O	<u>1.10</u>	(0/-)
As_O	<u>0.90</u>	
P_O	<u>0.70</u>	
N_O	<u>0.40</u>	

VBM

Large size mismatched p-type doping in ZnO:As

The new model:

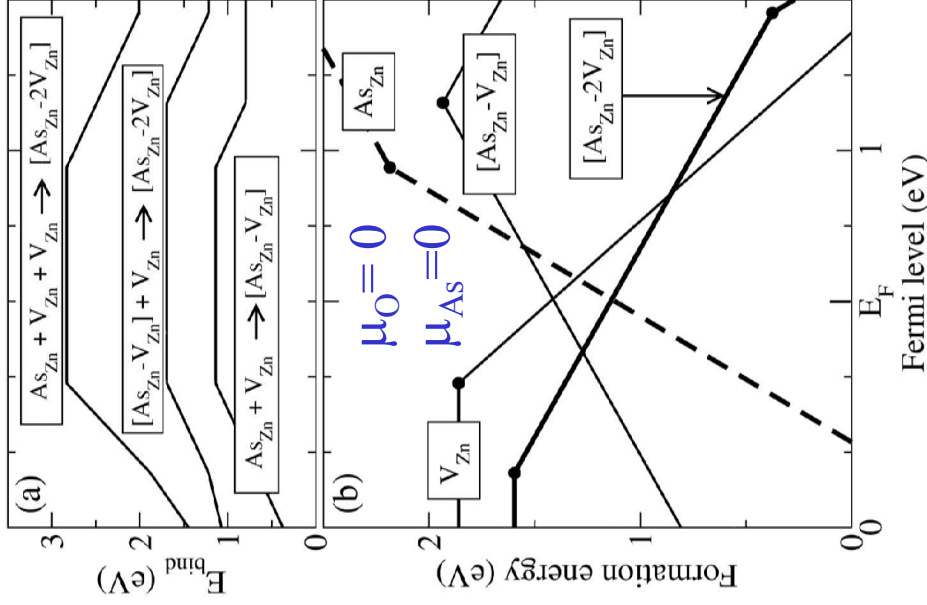
- Atomic size of As and Zn are similar
- As_{Zn} has relatively lower formation energy but it is a (triple) donor
- V_{Zn} is a native (double) acceptor with low formation energy
- One As_{Zn} and two V_{Zn} bind strongly and form a new acceptor complex ($\text{As}_{\text{Zn}}\text{-}2\text{V}_{\text{Zn}}$)
- The complex has low formation energy and low ionization energy (~ 150 meV)



[$\text{As}_{\text{Zn}}\text{-}2\text{V}_{\text{Zn}}$ complex]

Large size mismatched p-type doping in ZnO:As

Calculated binding energy and defect formation energy for various As-related defect complexes in ZnO

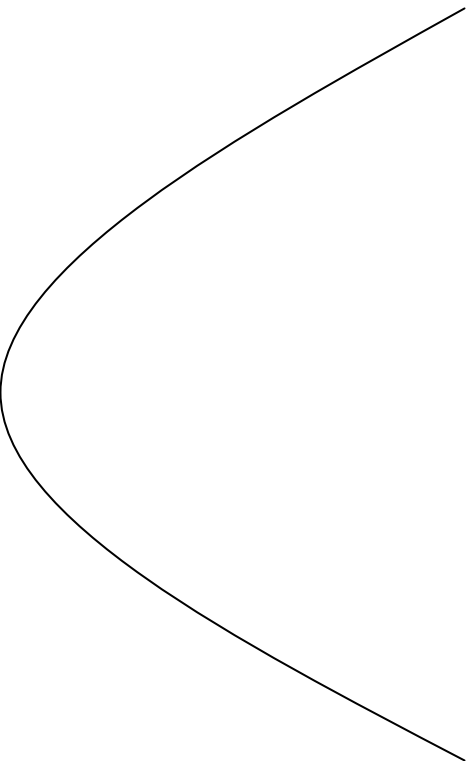


- Strong Coulomb interaction and strain compensation lowers the formation energy of the $\text{As}_{\text{Zn}}-2\text{V}_{\text{Zn}}$ defect complex
- Coupling between the As_{Zn} donor states and the V_{Zn} acceptor states lowers the ionization energy of the complex relative to V_{Zn}



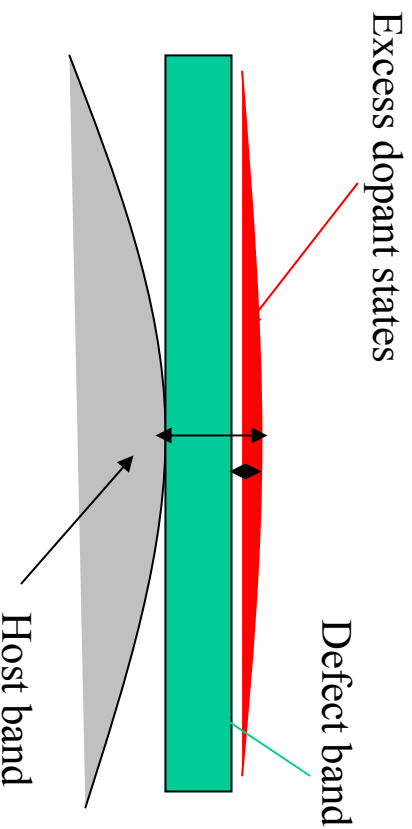
Modify the host band structure to reduce ionization energy and compensation

Universal approach to overcome the doping asymmetry in wide-band-gap semiconductors

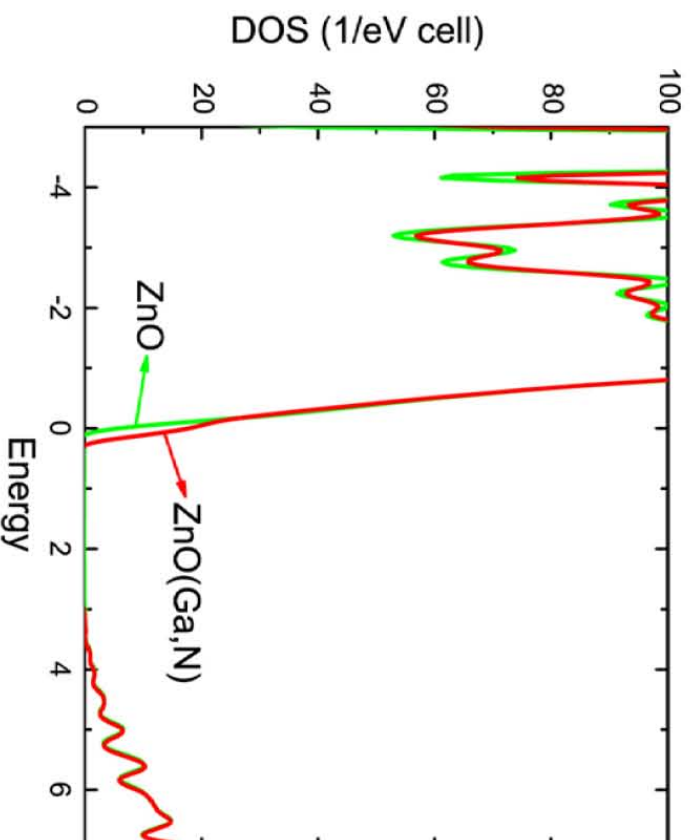


➤ First, through effective doping of mutually **passivated defect pairs**, we introduce a fully compensated defect band near the VBM or CBM of the host

➤ Second, after the fully compensated insulating phase is formed, use **excess dopants** to dope the passivated system by ionizing the defect band

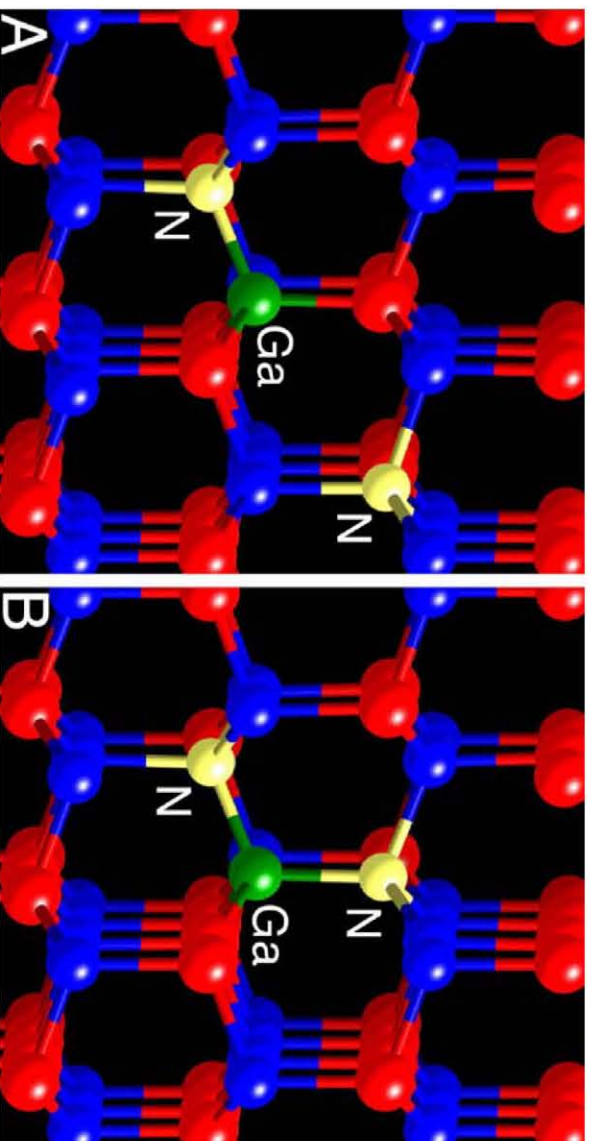


Modify the valence band edge of ZnO by passivate doping of Ga with N



- N combined with Ga creates a passivated defect band above the host ZnO VBM

Create shallow acceptor level by doping the
passivated ZnO:(Ga+N) system using
excess N



- The calculated defect level of N is about 0.1 – 0.2 eV above the defect band

Possible dopants or dopant complexes for p-type doping in ZnO

- Based on defect wavefunction analysis, various microscopic models have been proposed to reduce the ionization energy of acceptor level in ZnO



- Doping of defect band is an effective and universal approach to doped wide band gap materials such as ZnO



Summary

We have analyzed the origin of p-type doping difficulty in ZnO.

Several strategies have been proposed to overcome the doping difficulty

- Increase defect solubility by “defeating” bulk defect thermodynamics using
 - optimized host elements chemical potential
 - surface enhanced defect solubility
 - molecular doping
 - large size-mismatched antisite doping
- Reduce defect ionization level by
 - combining donor with acceptor to modify defect wavefunctions
 - reducing p-d coupling between defect level and host states
- Design new dopable materials by adjusting the band edges states using passivated doping and subsequent doping using the same dopants



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