Ultra Wide Bandgap Semiconductors and Interfaces for High Power Electronics

Robert J. Nemanich[1], Stephen Goodnick[1], Srabanti Chowdhury[3],

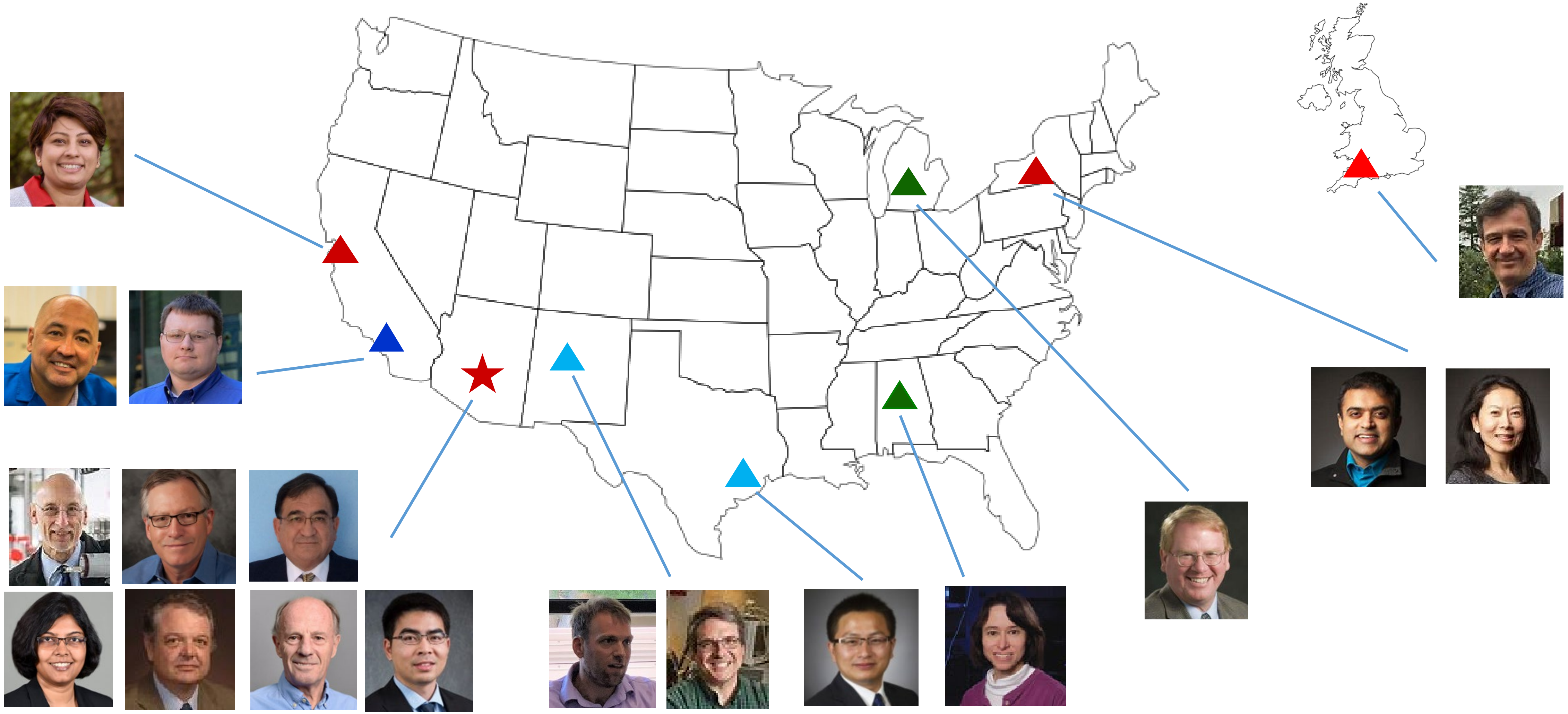
[1]Arizona State University; [2]Stanford University;

U.S. DEPARTMENT OF ENERGY | Office of Science

Ultra Materials for a Resilient, Smart Electricity Grid (ULTRA)

Director: Robert Nemanich, Deputy Director: Steve Goodnick,
Research Collaborations Director: Srabanti Chowdhury

ULTRA



Arizona State University

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Sandia National Laboratories

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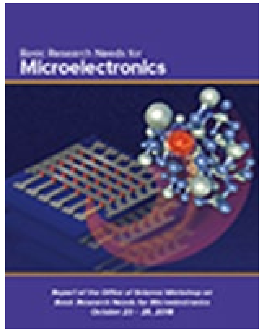
DOE Report: Basic Research Needs for Microelectronics

PRD 5 Reinvent the electricity grid through new materials, devices, and architectures



Two of five transformers in transmission substation, Melbourne, Australia

Potentially 100 lbs, Solid-State Transformer

Enabled by
- Ultra semiconductors
  - Wide bandgap
  - Low elect. resistance
  - Thermally conductive
- Solid state transformers

Figure 6. “Substation in a suitcase” and analogy with the miniaturization progress for digital computation. Courtesy of Jerry Simmons, Sandia National Laboratories.

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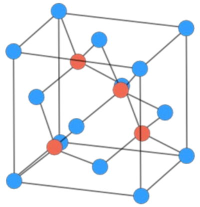
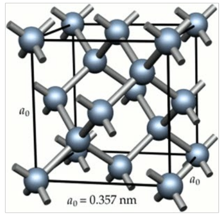
ULTRA

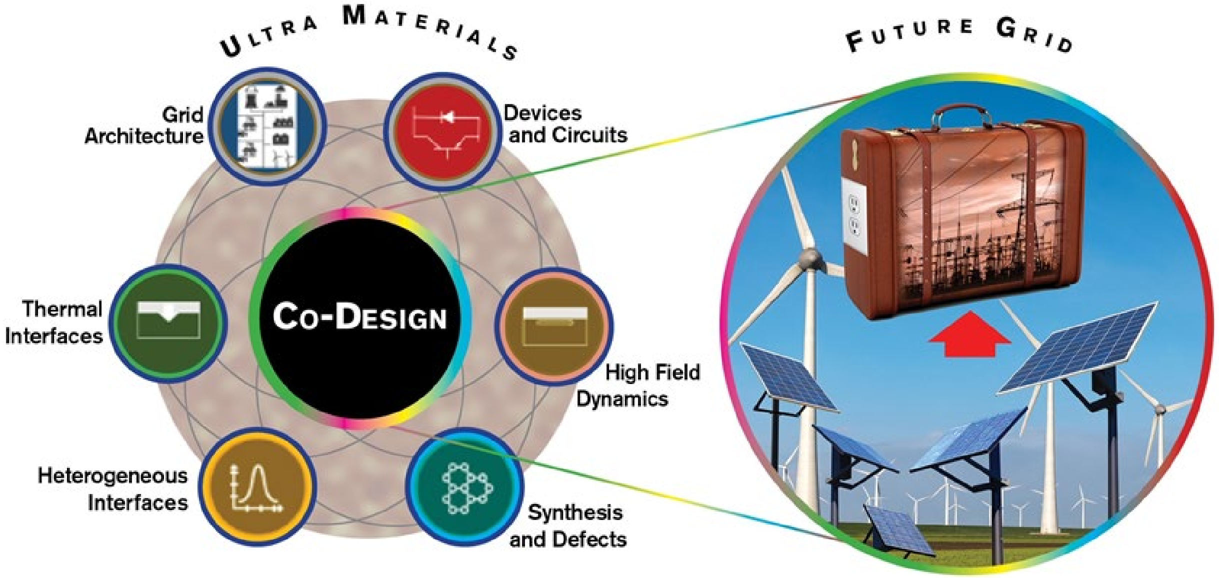
Wurtzite AlN

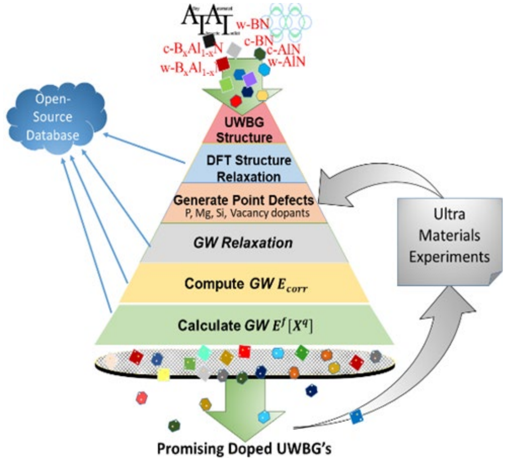


Cubic boron nitride (c-BN)



Diamond Cubic





To achieve extreme electrical properties and phenomena through fundamental understanding of ultra wide bandgap materials, which will enable a resilient, smart electricity grid.

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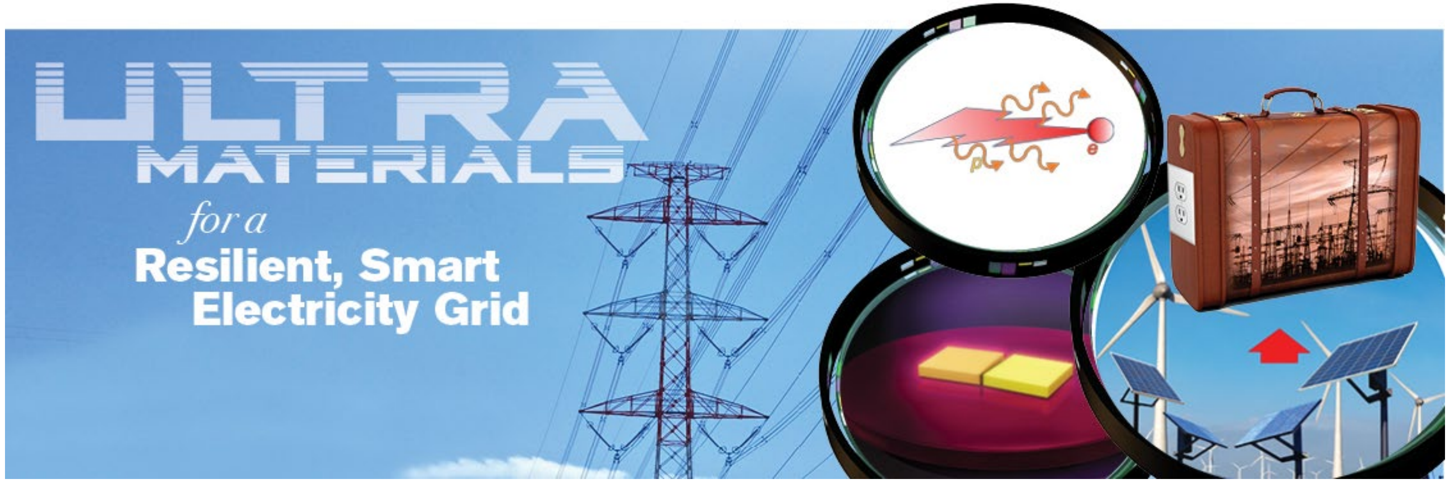
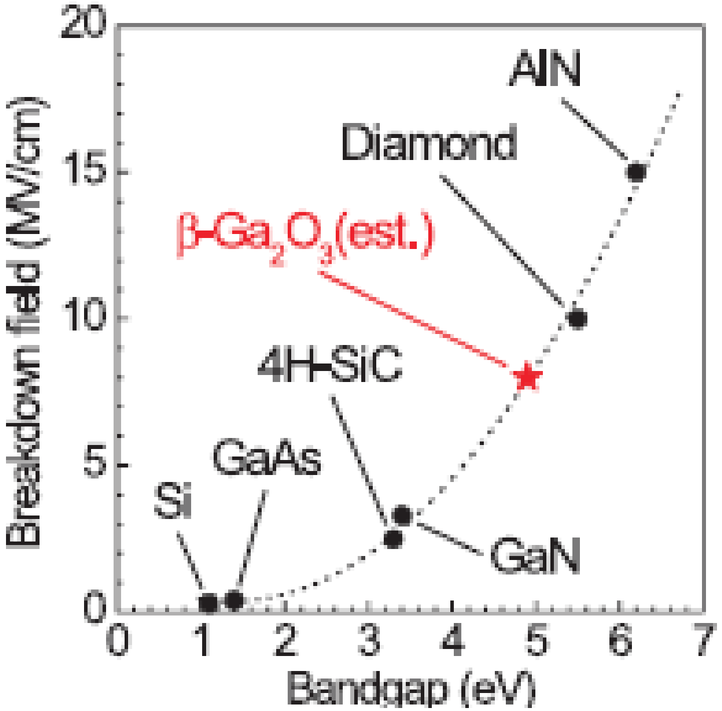
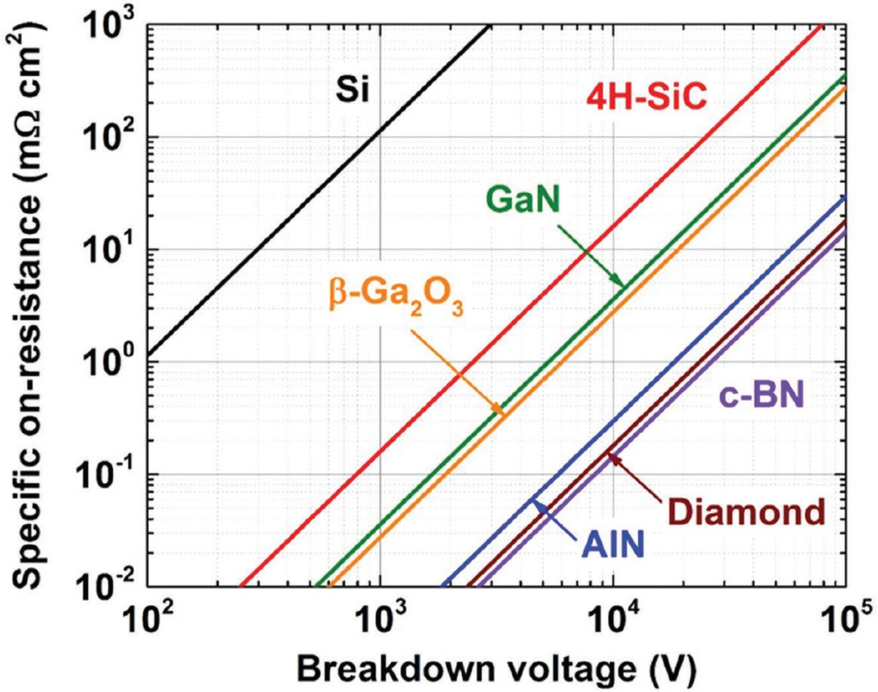


Co-Design questions drive ULTRA EFRC's work:

1. How can we achieve breakdown fields greater than 10 MV/cm?
2. How can we achieve current densities greater than 100,000 A/cm^2 and conduct the heat away?
3. What new phenomena and device configurations will enable efficient systems?
4. What electricity grid architecture will efficiently support the diverse needs of a fully electrified society?

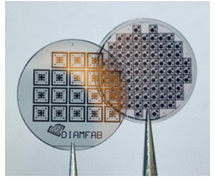
Wide Bandgap Properties



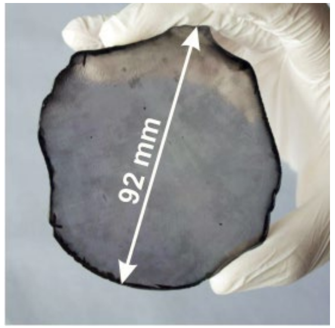


Gallium oxide (Ga_2O_3) metal-semiconductor field-effect transistors on single-crystal beta-Ga_2O_3 (010) substrates, M Higashiwaki et al, APL 100, 013504 (2012)
Ultrawide-Bandgap Semiconductors: Research Opportunities and Challenges, J. Tsao et al., Adv. Electron. Mater. 2017, 1600501. DOI: 10.1002/aelm.201600501

ULTRA Semiconductors

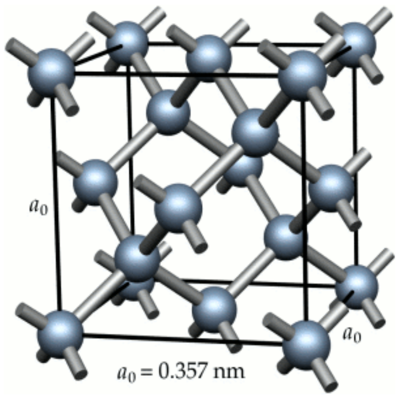


DiamFab



Augsburg Univ.

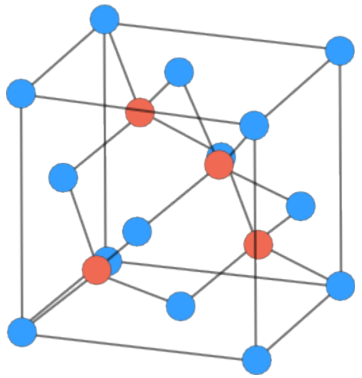
Diamond Cubic



- sp^3 bonded carbon
- C – 6e
- Diamond Cubic

a = 3.57 Å

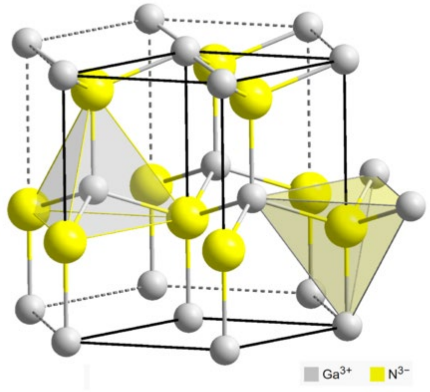
Cubic Boron Nitride (c-BN)



- sp^3 bonded BN
- B - 5e; N – 7e
- Zinc Blende

a = 3.62 Å[2]

Wurtzite AlN ($B_xAl_{1-x}N$)

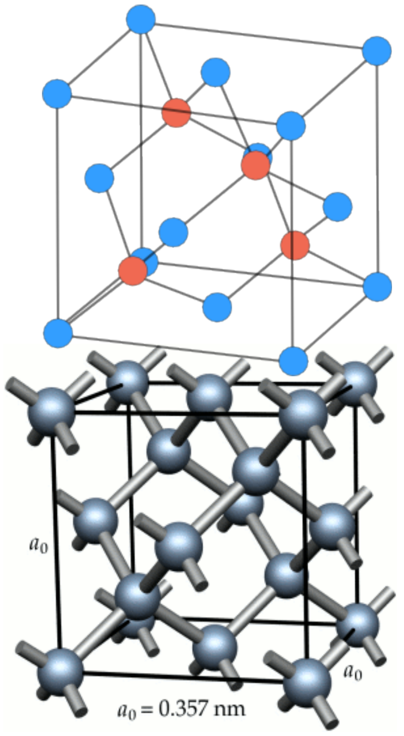


- sp^3 bonded Al-N
- Al - 13e; N – 7e
- Wurtzite structure
- a = 3.11 Å
- c = 4.93 Å

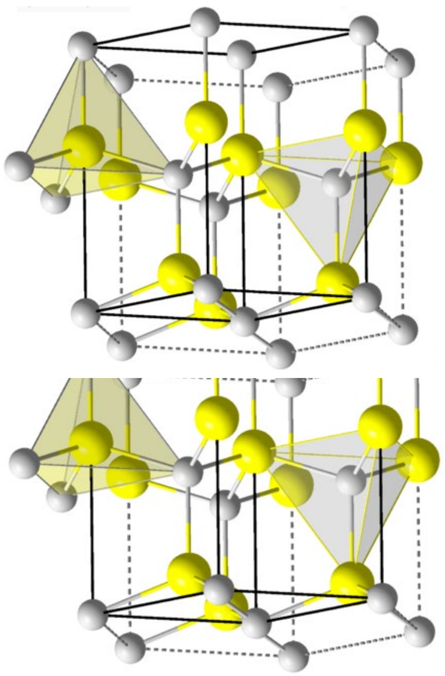
HexaTech
50 mm

G. L. Doll, J. A. Sell, C. A. Taylor II, and R. Clarke, Phys. Rev. B, **43**, 6816 (1991).

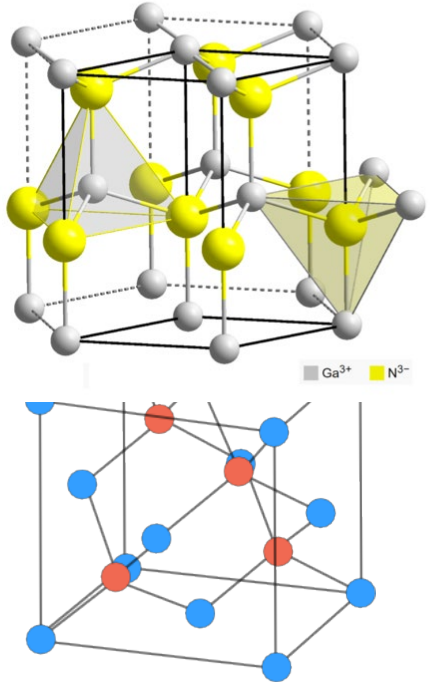
ULTRA Semiconductor Interfaces



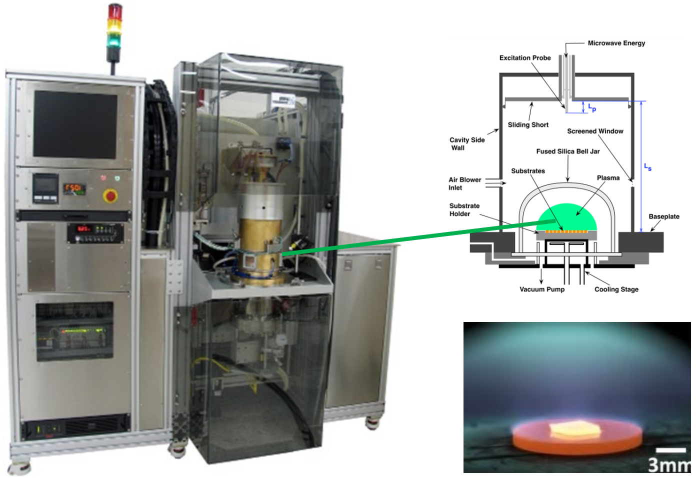
Interface Chemistry
c-BN / diamond
III-V / IV



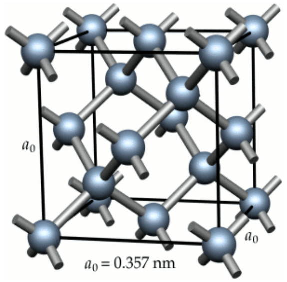
Interface Polarization
AlN / BAlN
Polar Wurtzite



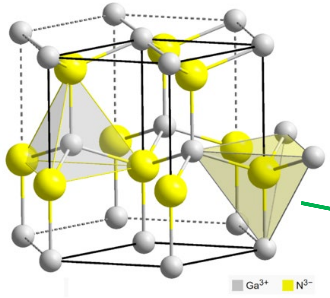
Interface Structure
c-BN / AlN
Zinc blende / Wurtzite
Cubic / Hexagonal



MPCVD

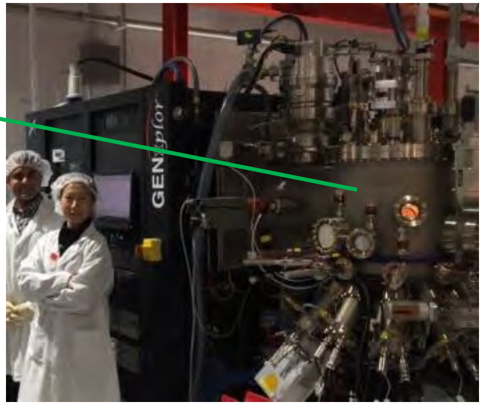


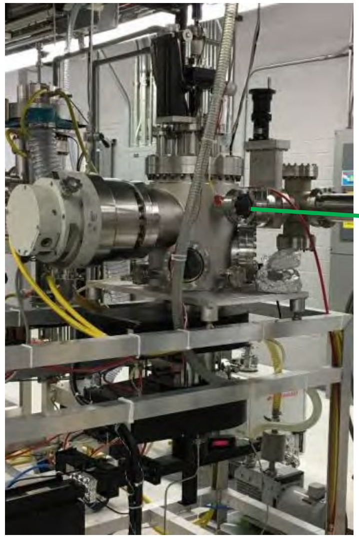
Diamond

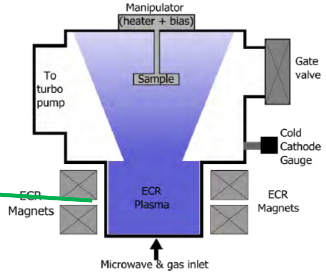


AlN and ($B_xAl_{1-x}N$)

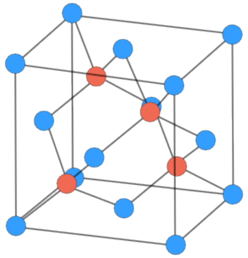
MBE



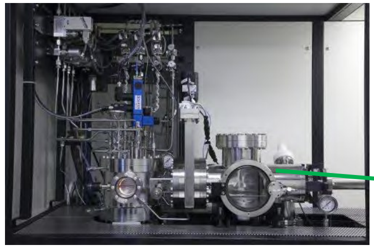




ECR-MPCVD

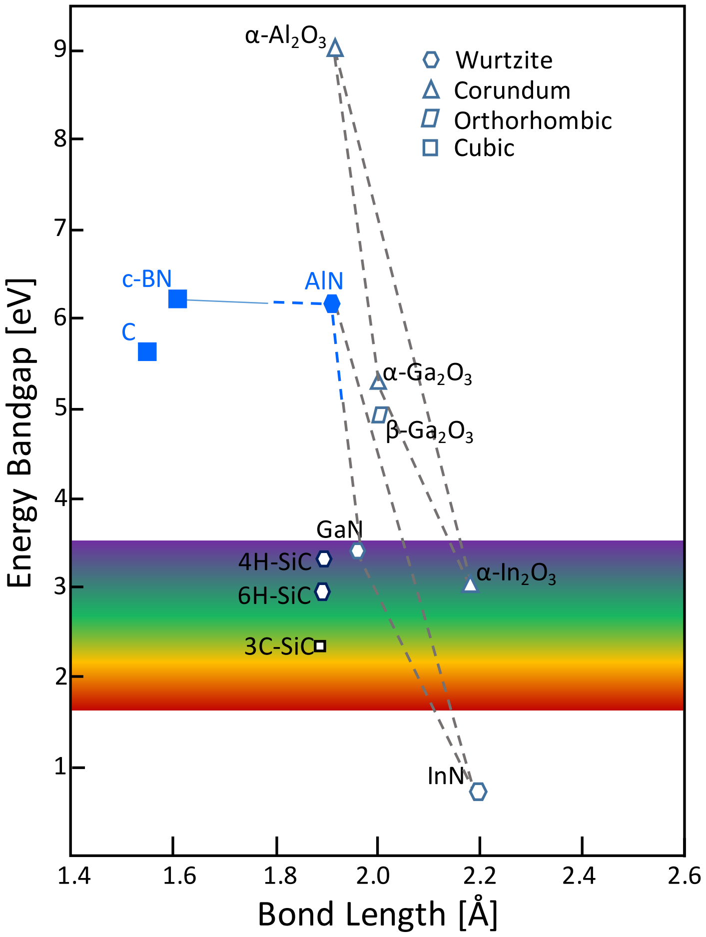


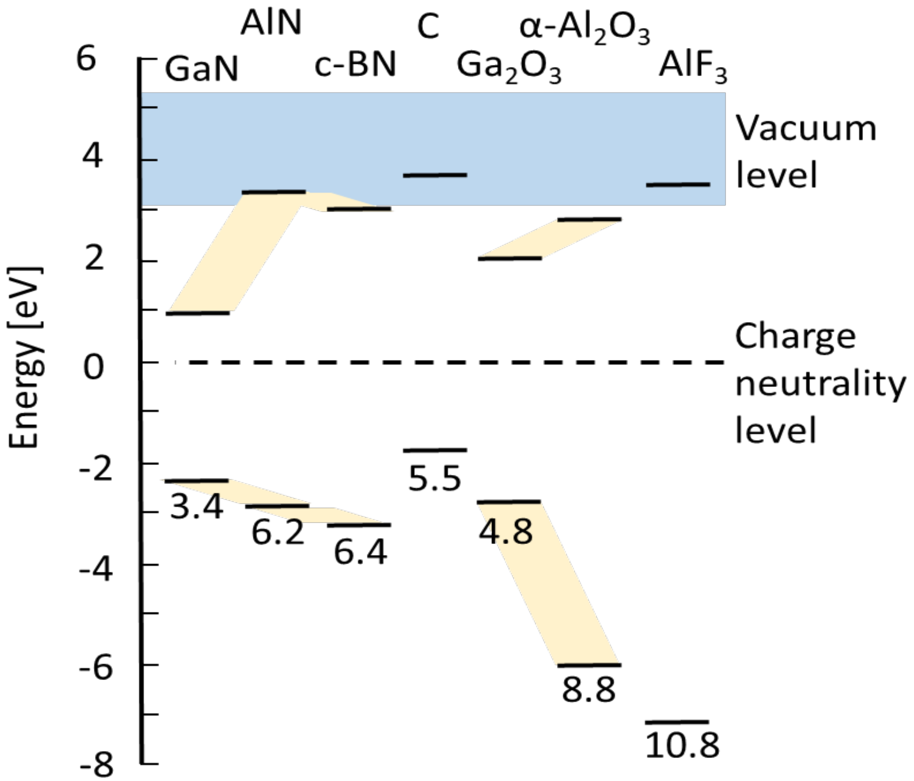
c-BN



MOCVD

ULTRA Materials

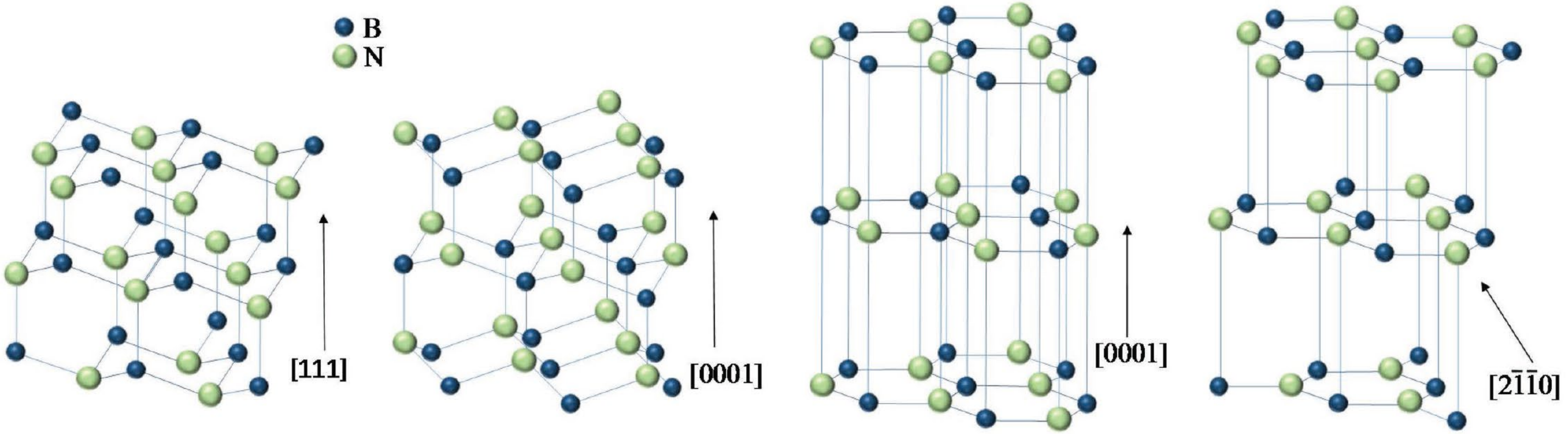




S. Fujita, JJAP 54, 030101 (2015)

c-BN and h-BN by PECVD
Chemical Properties Control

Boron Nitride Crystalline Phases

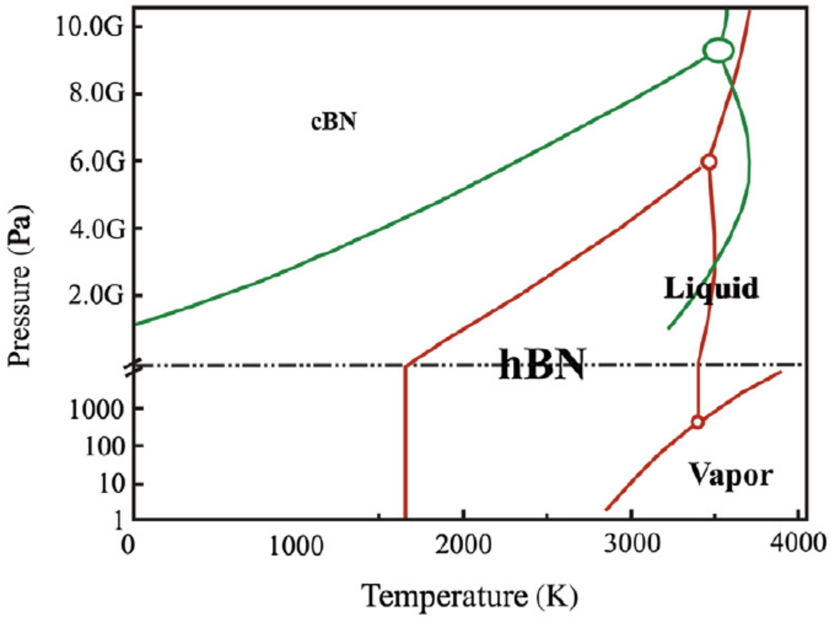


(a) Cubic BN (b) Wurtzite BN (c) Hexagonal BN (d) Rhombohedral BN

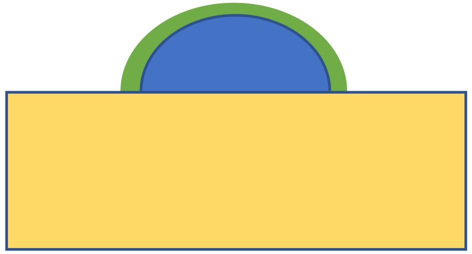
Density (gm/cm^3)-	3.48	3.47	2.2	2.26
Bonding	sp^3	sp^3	sp^2	sp^2

N. Izyumskaya et al., Adv. Electron. Mater. 3, 1600485 (2017)

Boron Nitride Crystalline Phases



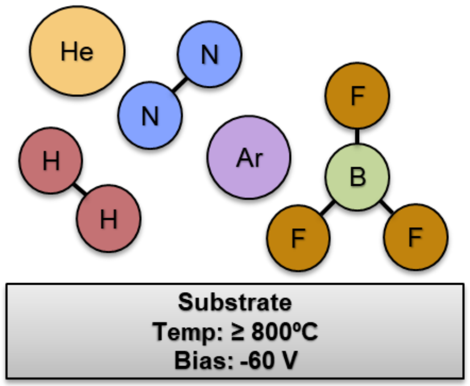
Green – Corrigan and Bundy 1975
Red – Solozhenko, Turkevich, Holzapfel (1999)



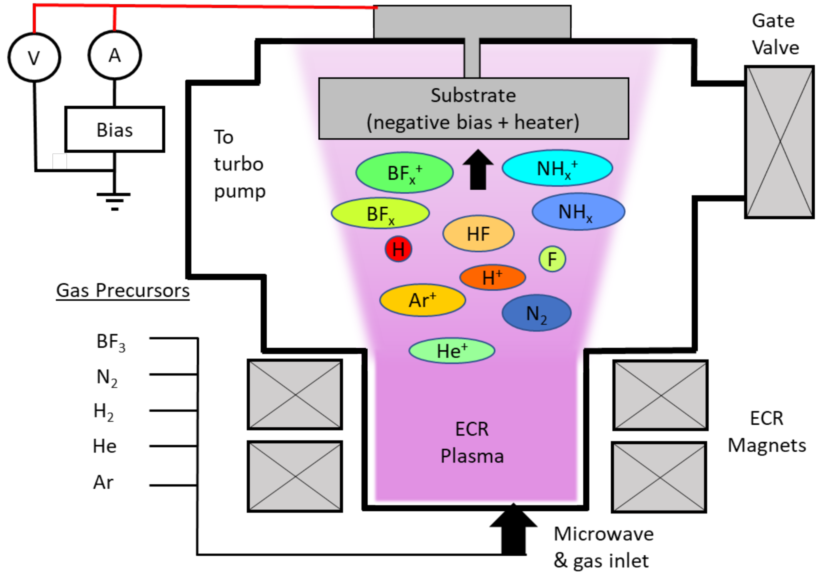
Surface energy increases
the energy for nucleation

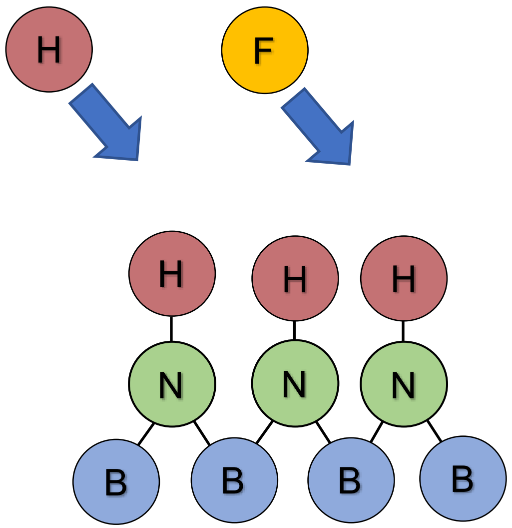
Wenjun Zhang et al., Comprehensive Hard Mater. (2018)
http://dx.doi.org/10.1016/B978-0-08-096527-7.00061-1

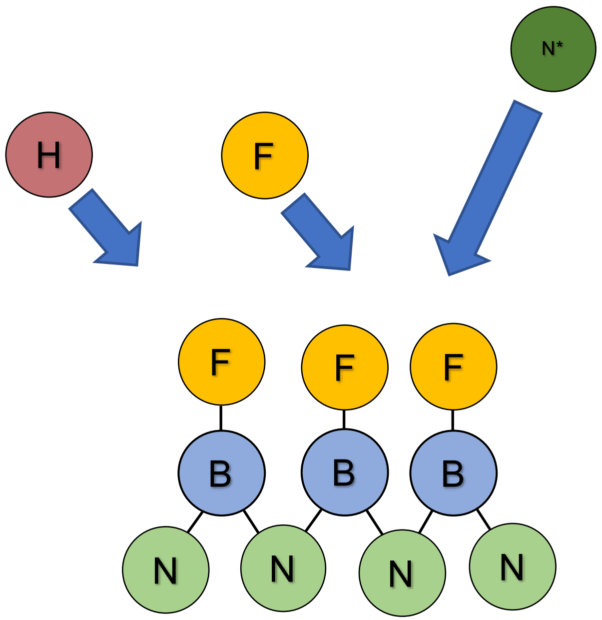
c-BN Growth



Substrate
Temp: ≥ 800ºC
Bias: -60 V







- H or F proposed for abstraction of H from N surface sites.
- H or F plus impinging ions proposed to abstract F from B surface sites.

Nucleation of Epitaxial c-BN

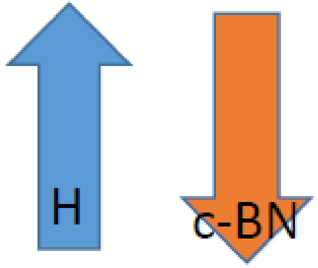
Precursors → **Plasma** → **Surface**

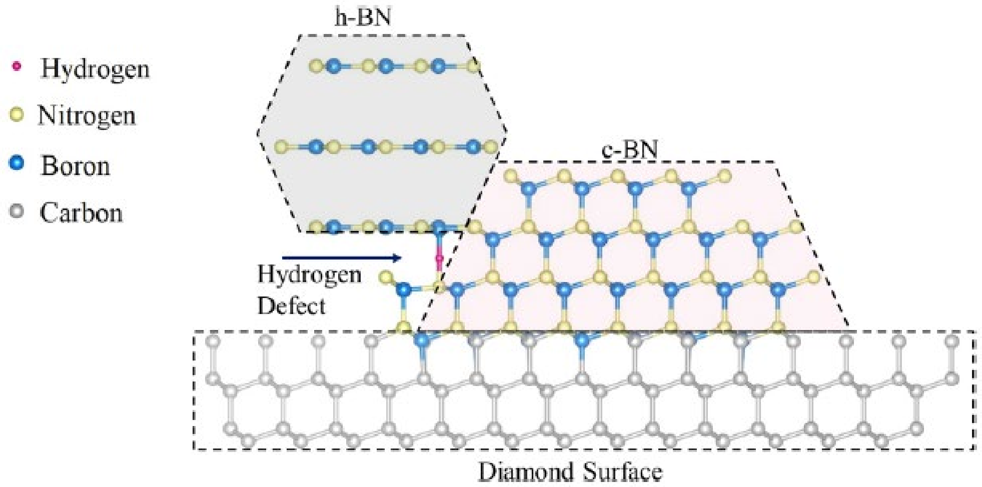
Ratio of H_2 to BF_3 is critical to the deposition of c-BN or h-BN

$$\text{Balanced: } 1.5H_2 + BF_3 + N_2 \rightleftarrows BF_x + NH_x + HF \rightleftarrows BN_{(s)} + (x+1)HF,$$

$$\text{Excess } H_2\text{: } 2H_2 + BF_3 + N_2 \rightleftarrows BF_x + NH_x + HF \rightleftarrows BN_{(s)} + (x+1)HF + H,$$

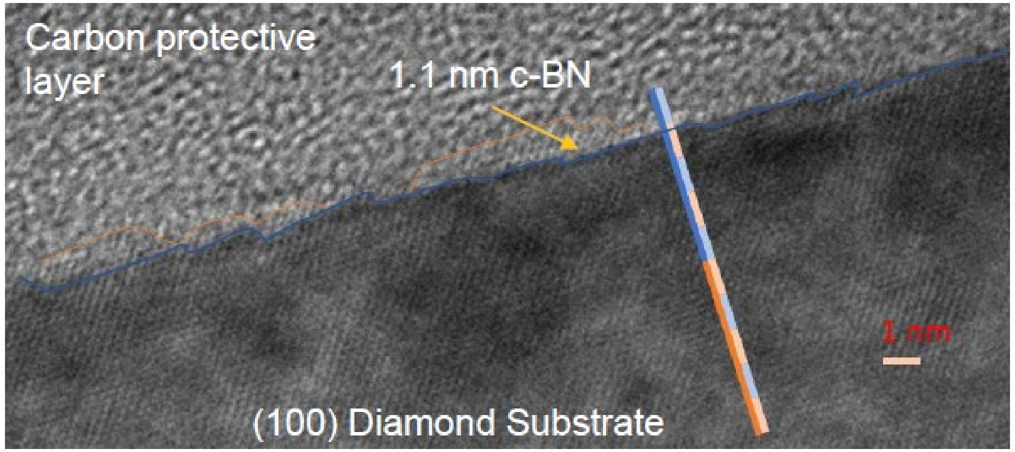
$$\text{Limited } H_2\text{:} 1H_2 + BF_3 + N_2 \rightleftarrows BF_x + NH_x + HF \rightleftarrows BN_{(s)} + (x+1)HF + F.$$





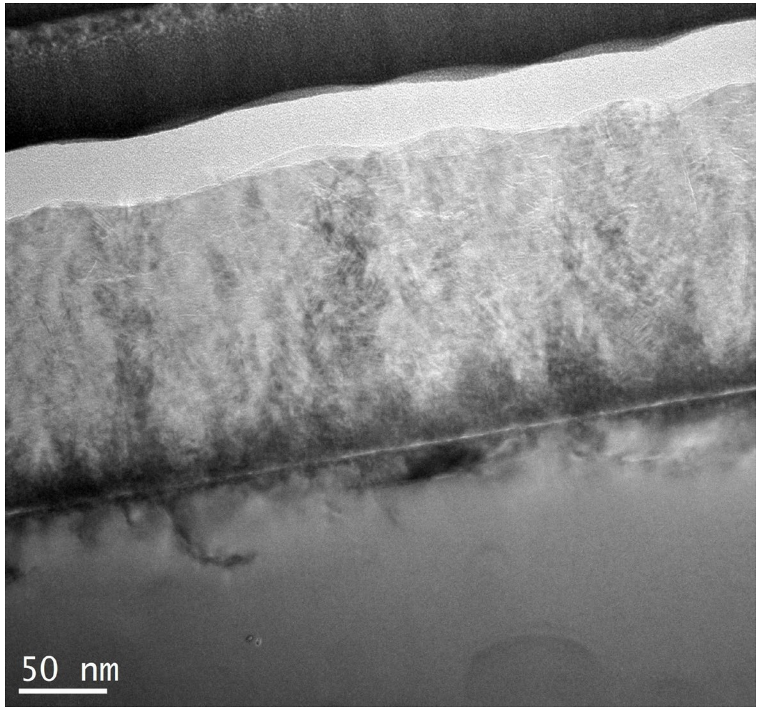
Hydrogen defects → h-BN

Transmission Electron Microscopy (TEM) Image

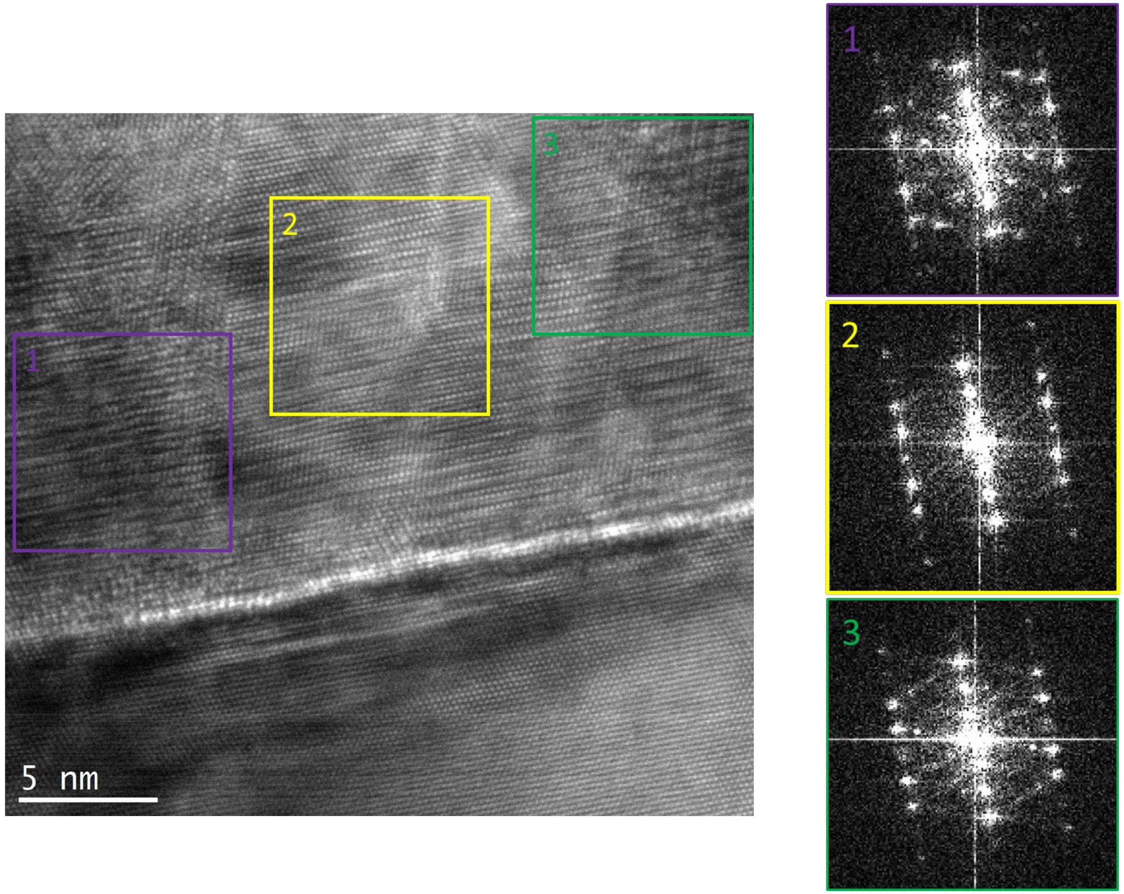


1. J. Brown, S. Vishwakarma, D. Smith, R. J. Nemanich, "Nucleation of cubic boron nitride on boron-doped diamond via plasma enhanced chemical vapor deposition", J. Appl. Phys 133, 215303 (2023)
2. D. Han *et al.*, "Role of hydrogen in the growth of boron nitride; cubic phase versus hexagonal phase", computational materials science 82, 310 (2014)
3. W. J. Zhang, C. Y. Chan, X.M. Meng, M.K. Fung, I. Bello, Y. Lifshitz, S.T. Lee and X. Jiang, "The Mechanism of Chemical Vapor Deposition of Cubic Boron Nitride Films from Fluorine-Containing Species," Angewandte Chemie Int. Ed., 44, 4749 (2005).

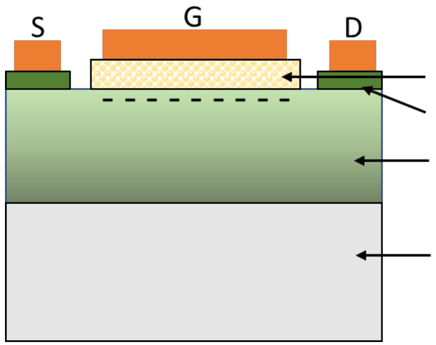
c-BN / w-BN – Diamond (111)



BN film thickness ~ 160 nm

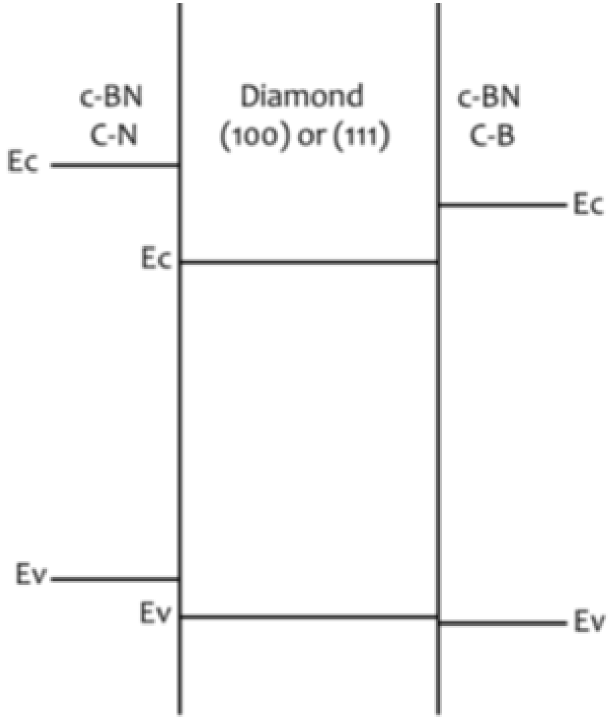


c-BN / h-BN – Diamond FETs



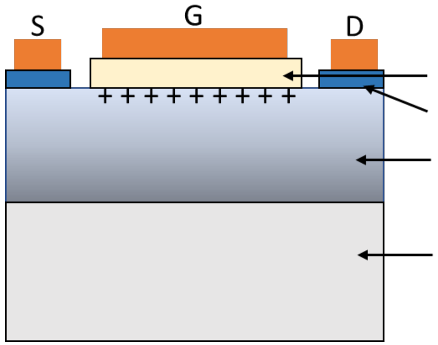
c-BN epitaxial layer
P-doped n+ diamond
P-doped n- diamond (graded)
Diamond substrate

n-channel



c-BN

h-BN

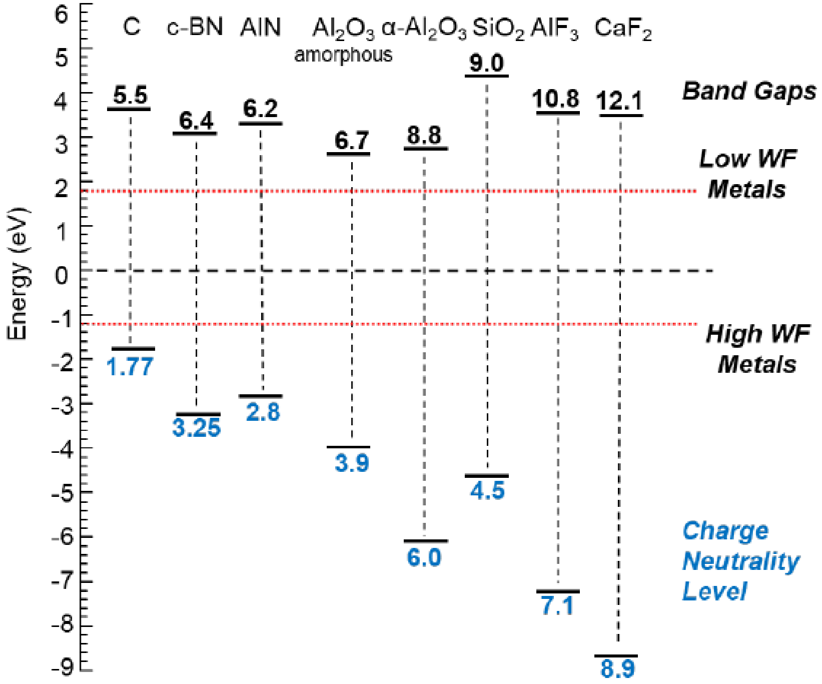


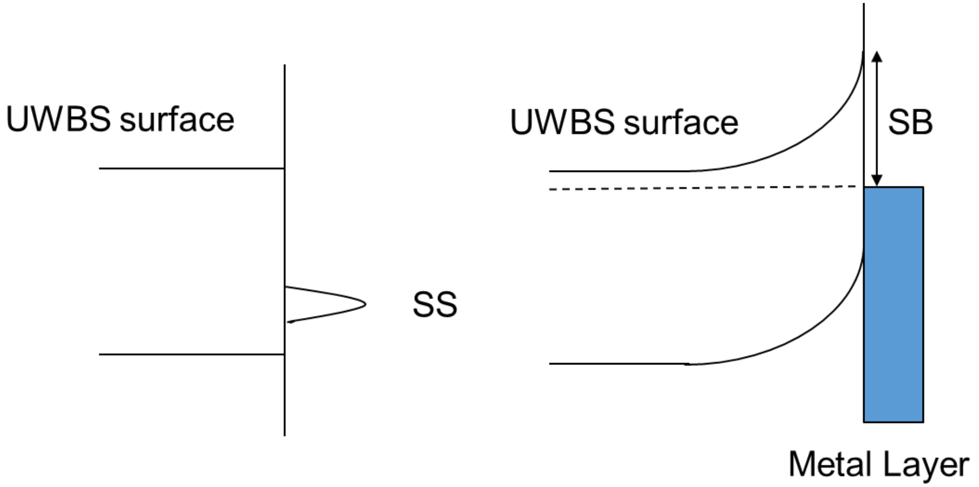
mp-BN dielectric layer
B-doped p+ diamond
B-doped p- diamond (graded)
Diamond substrate

p-channel

Electrical Contacts
Interface states control

Electron Contacts to UWBS

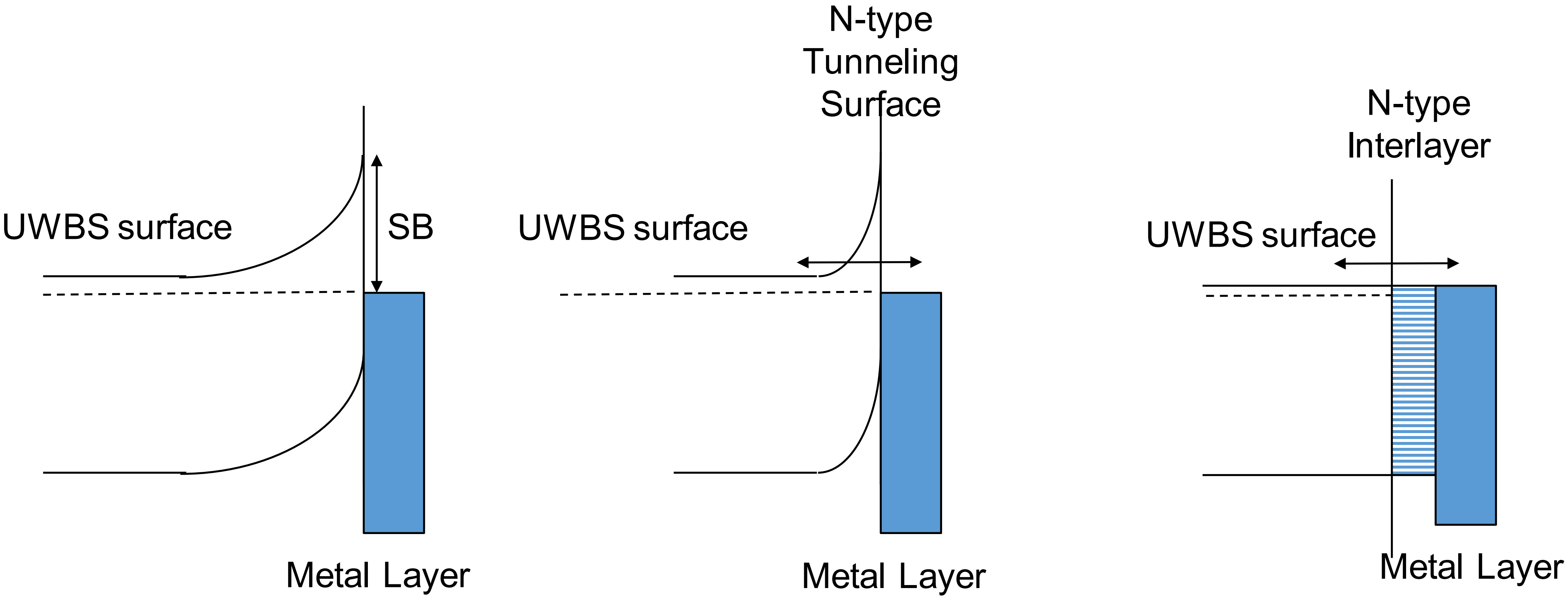




Low work function contacts to n-type UWBS is complicated

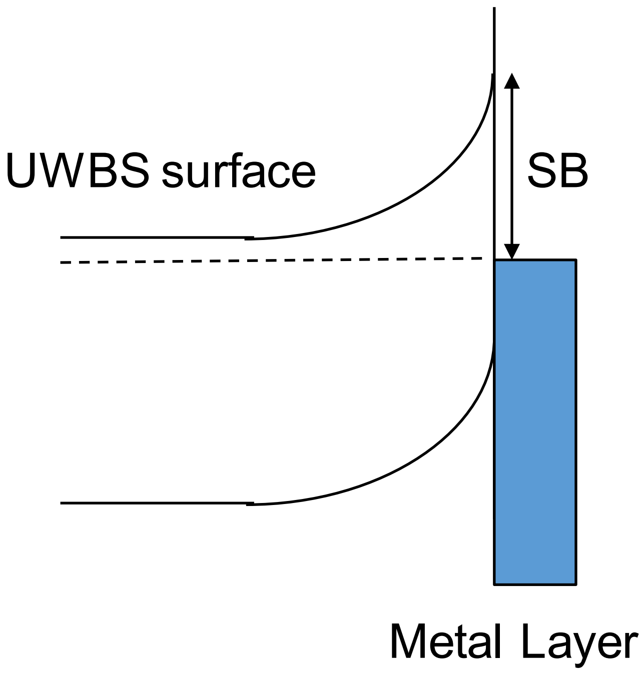
Surface states (or CNL) on diamond and AlN (and c-BN) can pin the interface Fermi level providing a large Schottky barrier that limits electron injection.

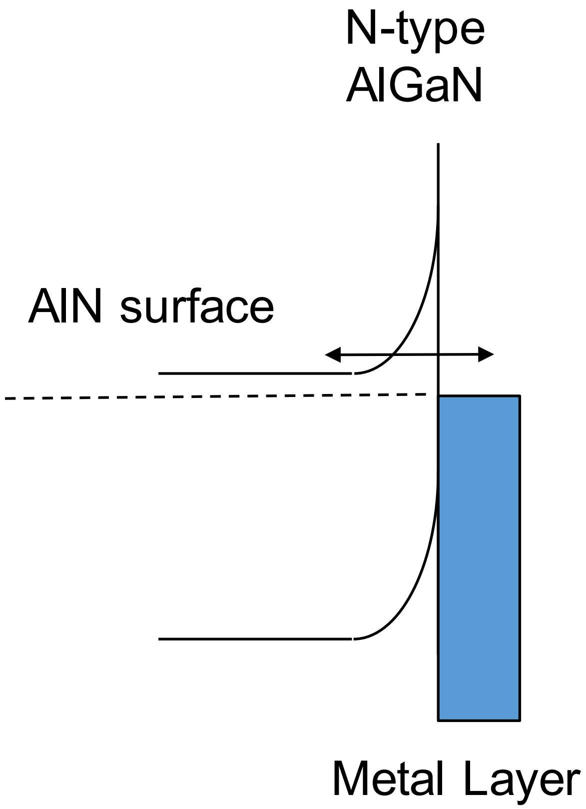
Electron Contacts to UWBS

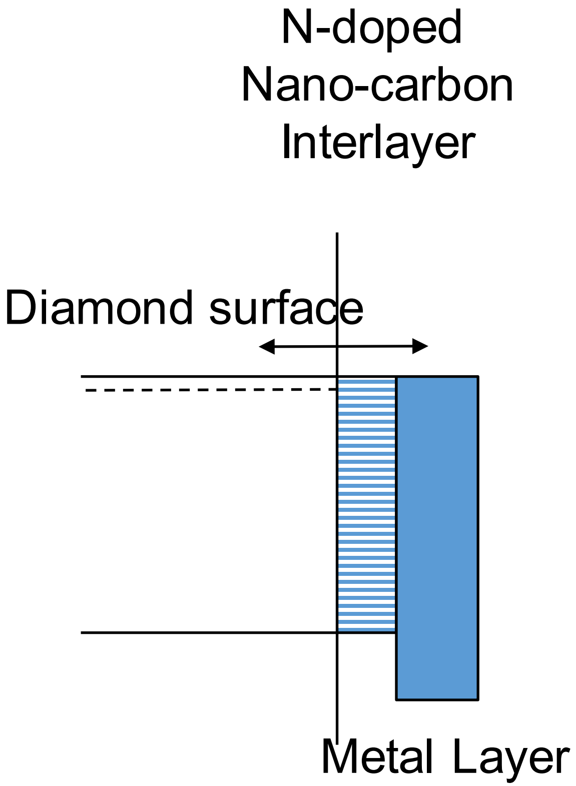


Low work function contacts to n-type UWBS is complicated

Electron Contacts to UWBS



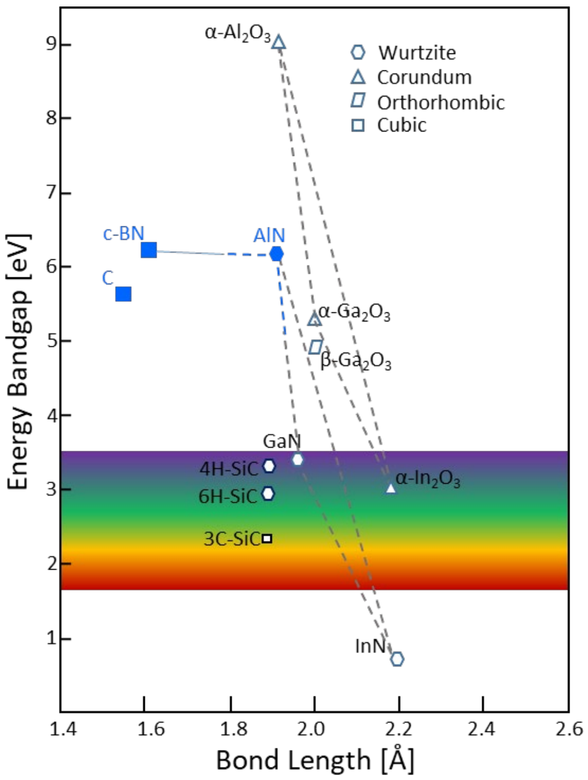


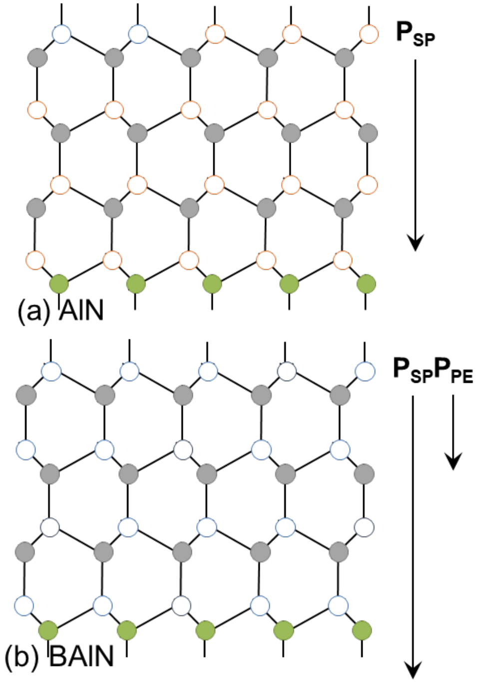


Low work function contacts to n-type
UWBS is complicated

Interface Doping
Polarization Discontinuity
Charge Transfer – Modulation Doping

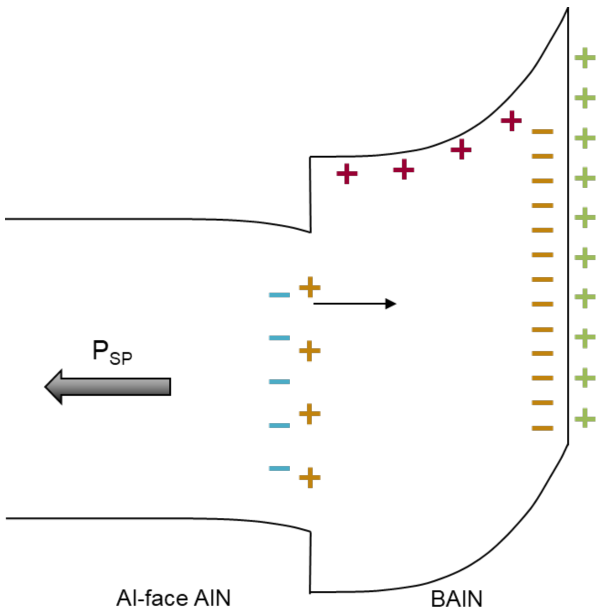
Polarization at AlN and BAlN interfaces





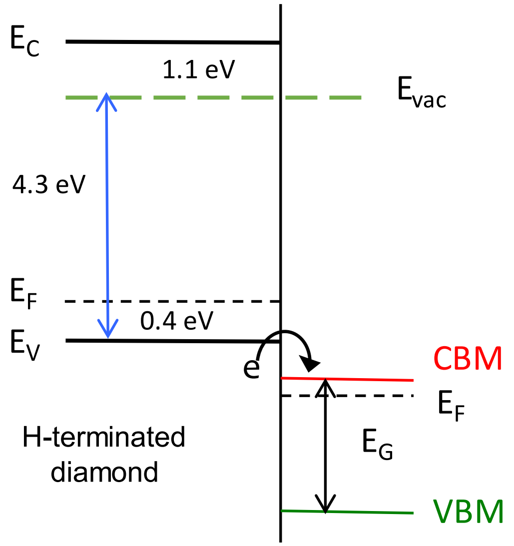
○ Ga (or Al) atoms

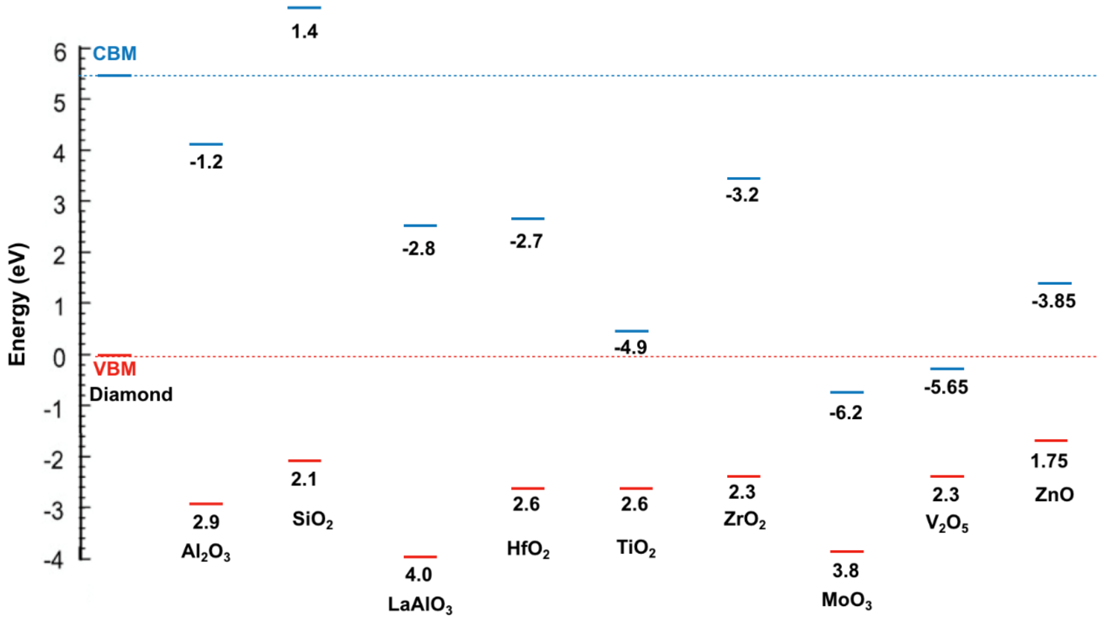
● N atoms



Charge Transfer in Other Dielectrics

Band Alignment of dielectrics on H-terminated diamond

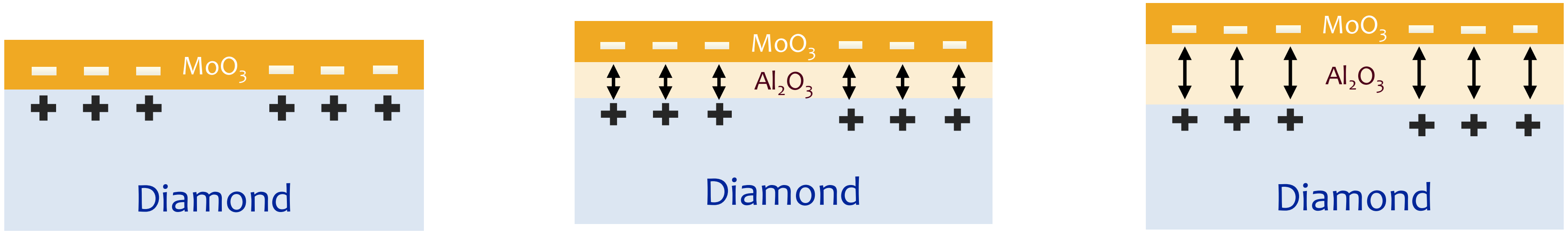




Band offset for dielectric on H-terminated diamond

Experimental Approach

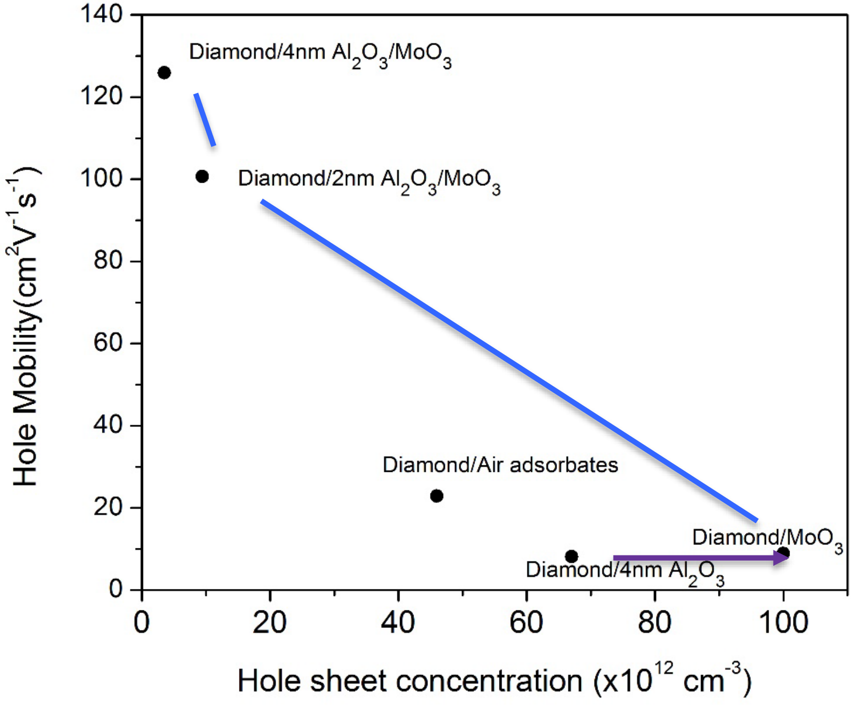
Surface transfer doping of diamond/Al_2O_3/MoO_3

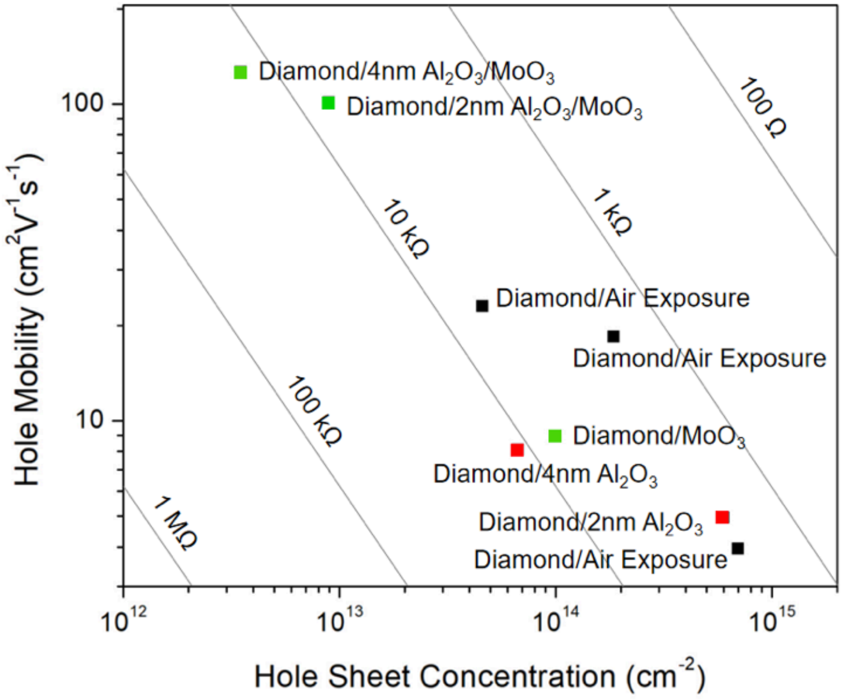


- Insert an interface layer to increase the distance between the hole accumulation layer in diamond and ions in acceptor layer.
- Reduce the ionic scattering and increase the hole mobility.

Diamond/Al_2O_3/MoO_3

Carrier Mobility and Concentration





Summary

Ultra wide bandgap semiconductors have been identified as crucial for a smart, resilient electricity grid.

ULTRA research is focused on 1) materials synthesis, defect reduction, doping, 2) interfaces and heterostructures, 3) electrical transport and 4) thermal transport.

Interfaces represent a unique challenge and opportunity to tune materials properties including electrical contacts, interface doping, and electronic band alignment.

Impacting power electronics can be enabled with a Co-design ecosystem focused on the future electricity grid.

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