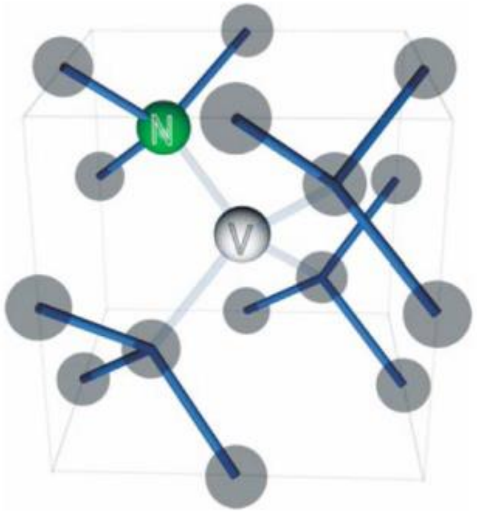
Surface termination effects for near-surface nitrogen-vacancy (NV) centers in diamond



Jyh-Pin Chou, Song Li, Alice Hu, and Adam Gali

Hungarian Academy of Sciences

香港城市大學
City University of Hong Kong

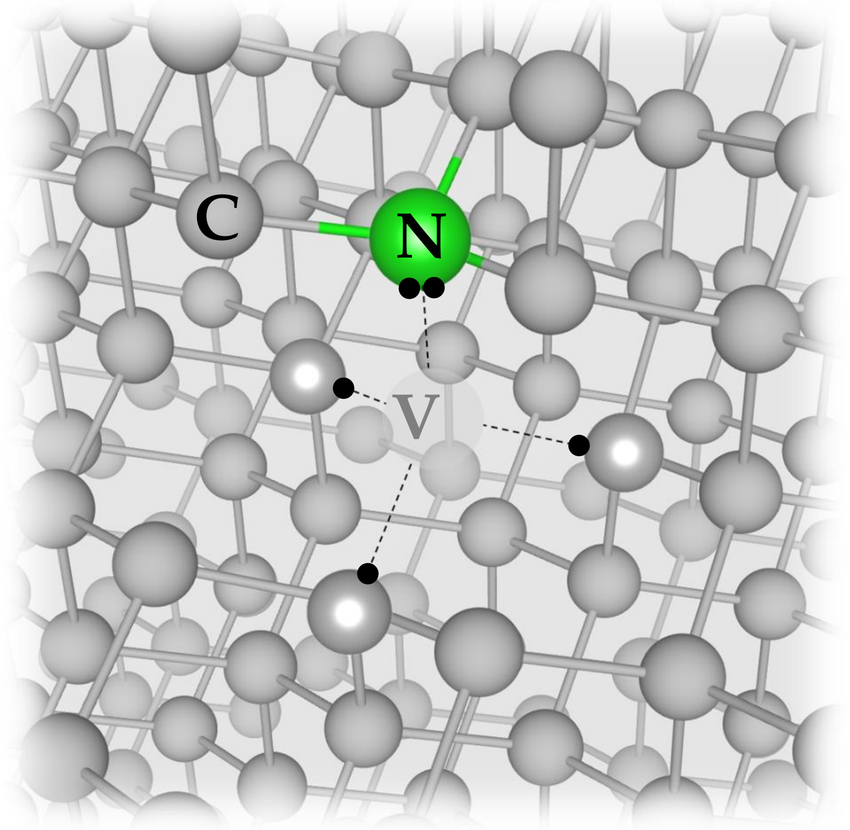
Nitrogen-Vacancy (NV) center in diamond

Diamond

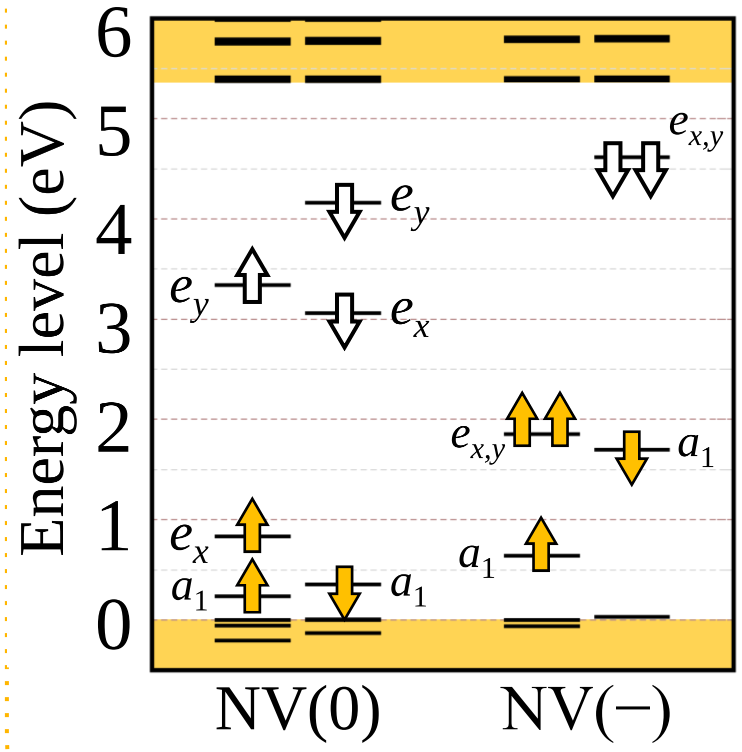
Chemical inertness
Radiation hardness
Wide bandgap (5.45 eV)

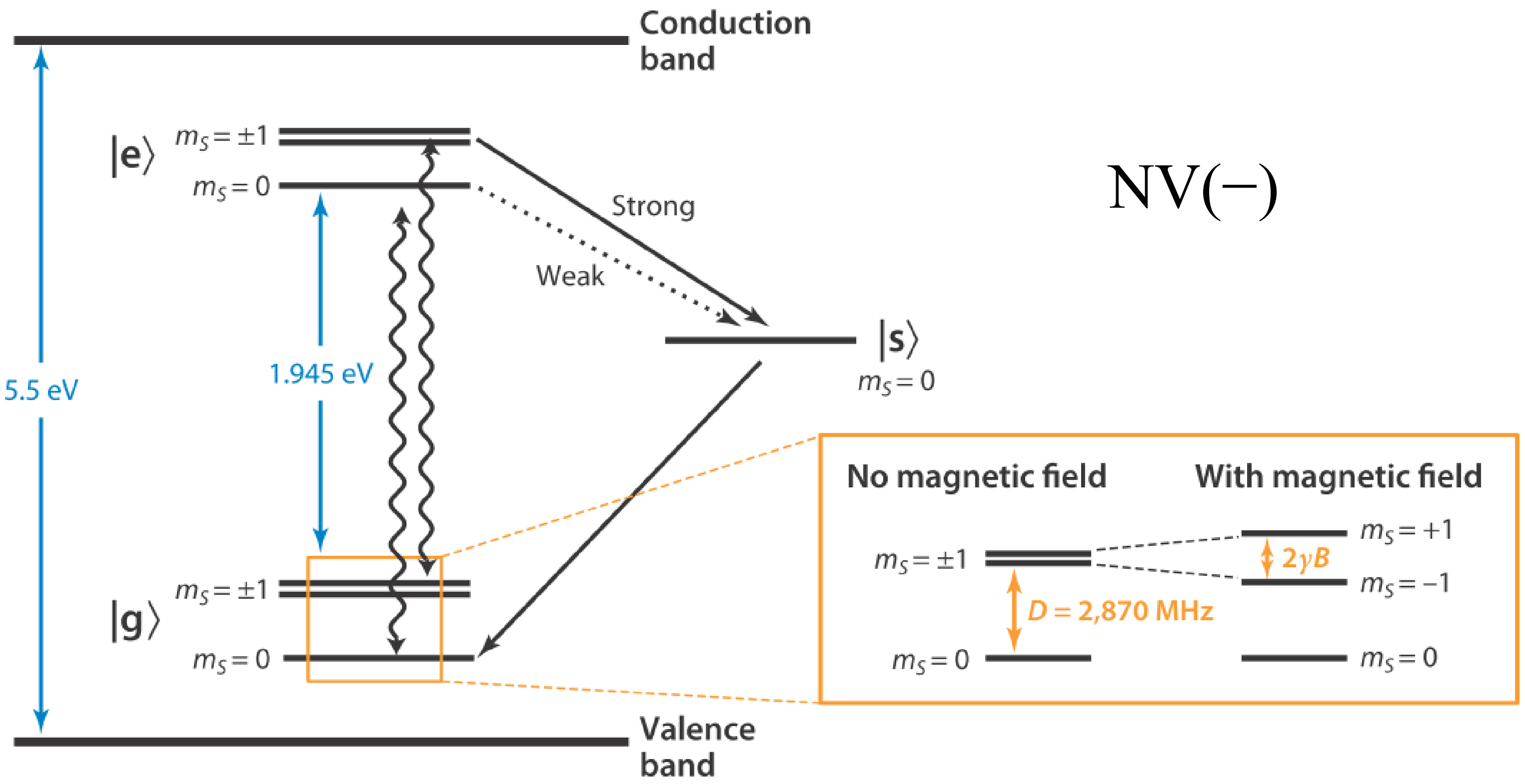
NV in diamond

Quantum bit (qubit)
Quantum sensing



Nitrogen-Vacancy (NV) center in diamond





NV(−)

Energy-level diagram of NV(−)

Annu. Rev. Phys. Chem. 2014. 65:83–105

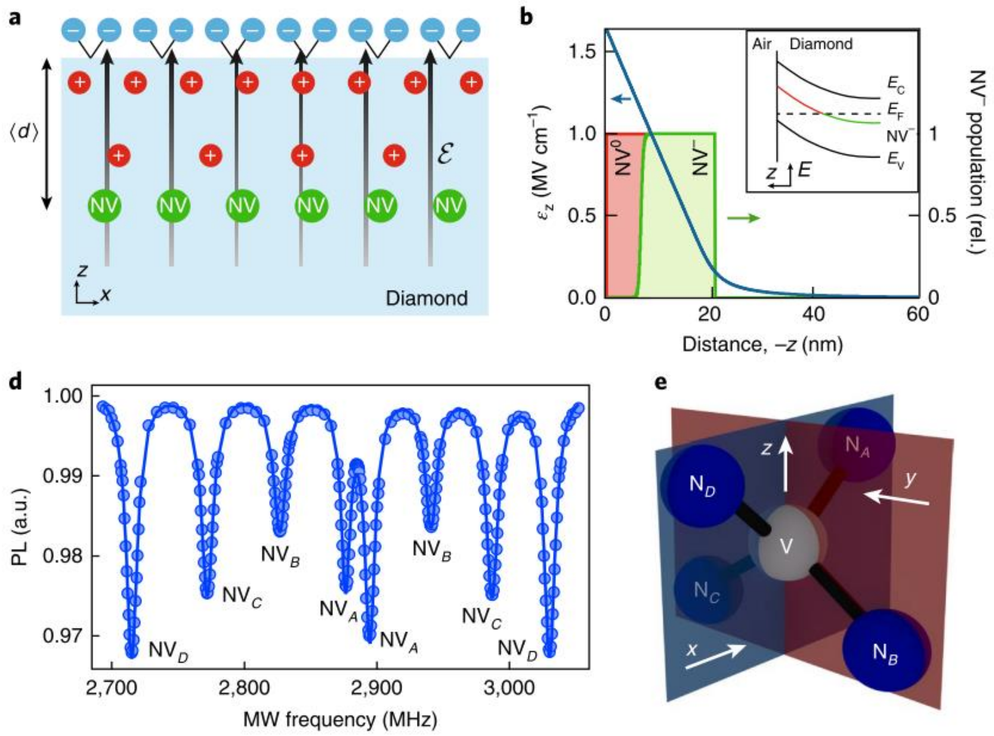
Quantum Sensing

ARTICLES
https://doi.org/10.1038/s41928-018-0130-0
nature electronics

Spatial mapping of band bending in semiconductor devices using in situ quantum sensors

D. A. Broadway[1,2,5], N. Dontschuk[1,2,5], A. Tsai[1], S. E. Lillie[1,2], C. T.-K. Lew[1,2], J. C. McCallum[1], B. C. Johnson[1,2], M. W. Doherty[3], A. Stacey[2,4], L. C. L. Hollenberg[1,2]* and J.-P. Tetienne[1]*

NATURE ELECTRONICS | VOL 1 | SEPTEMBER 2018 | 502–507



ELECTRIC FIELD SENSING

Quantum Sensing

LETTER

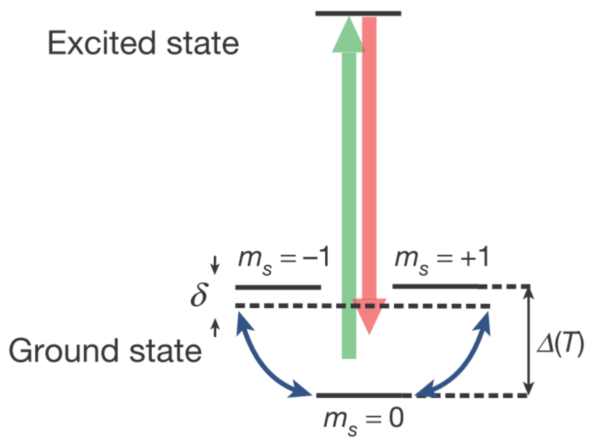
doi:10.1038/nature12373

Nanometre-scale thermometry in a living cell

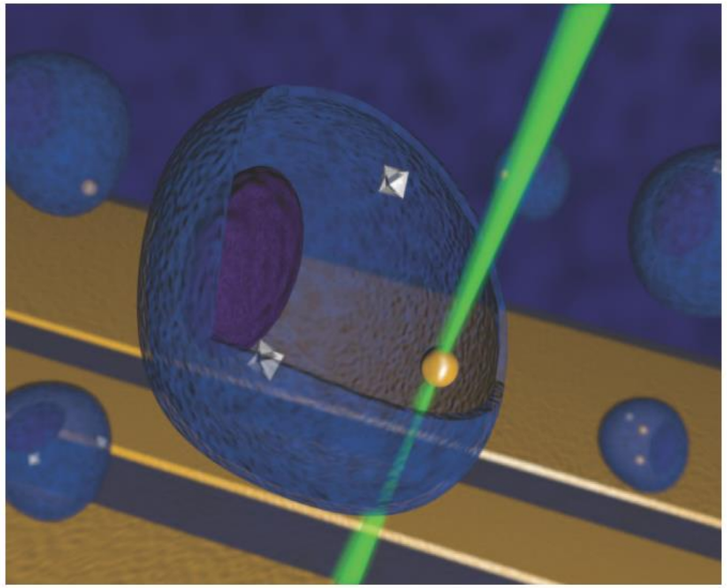
G. Kucsko[1]*, P. C. Maurer[1]*, N. Y. Yao[1], M. Kubo[2], H. J. Noh[3], P. K. Lo[4], H. Park[1,2,3] & M. D. Lukin[1]

TEMPERATURE SENSING

b



a



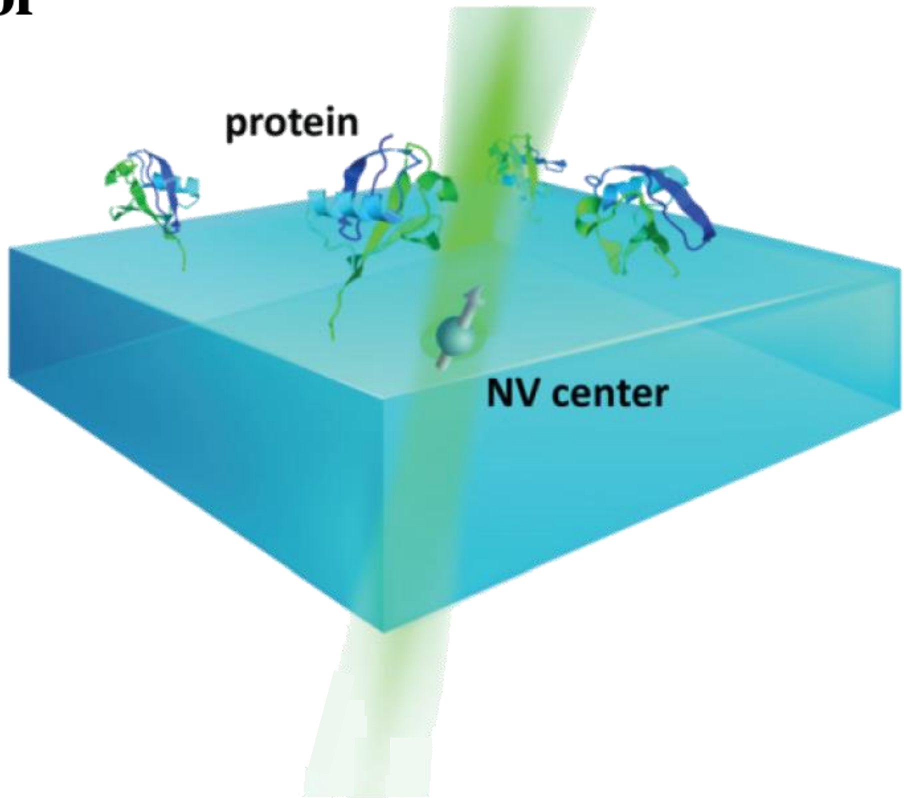
Quantum Sensing

Science REPORTS

Cite as: I. Lovchinsky *et al.*, *Science* 10.1126/science.aad8022 (2016).

Nuclear magnetic resonance detection and spectroscopy of single proteins using quantum logic

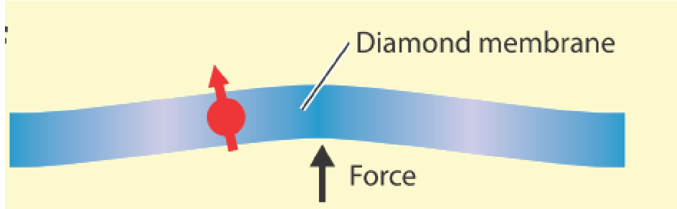
I. Lovchinsky,[1] A. O. Sushkov,[1,2]* E. Urbach,[1] N. P. de Leon,[1,2] S. Choi,[1] K. De Greve,[1] R. Evans,[1] R. Gertner,[2] E. Bersin,[1] C. Müller,[3] L. McGuinness,[3] F. Jelezko,[3] R. L. Walsworth,[1,4,5] H. Park,[1,2,5,6]† M. D. Lukin[1]†

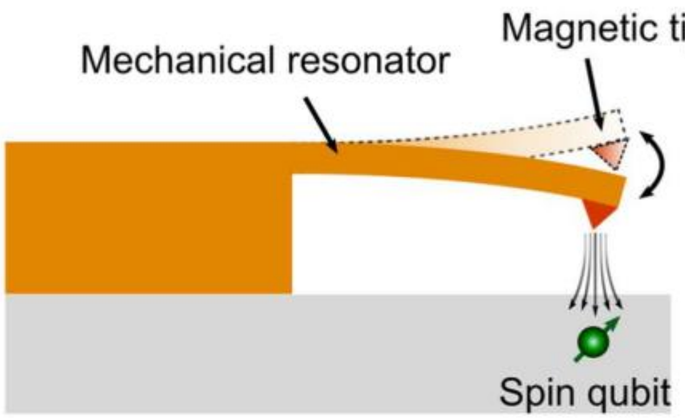


<u>High-confidence detection of individual protein and reveal information about their chemical composition.</u>

Quantum Sensing

To maximum the sensibility, NV sensor should be placed as close as possible to the surface; the surface morphology becomes critical!





Magnetic coupling

J. Opt. 19 (2017) 033001

Nitrogen-Vacancy Centers in Diamond: Nanoscale Sensors for Physics and Biology

Romana Schirhagl, Kevin Chang, Michael Loretz, and Christian L. Degen

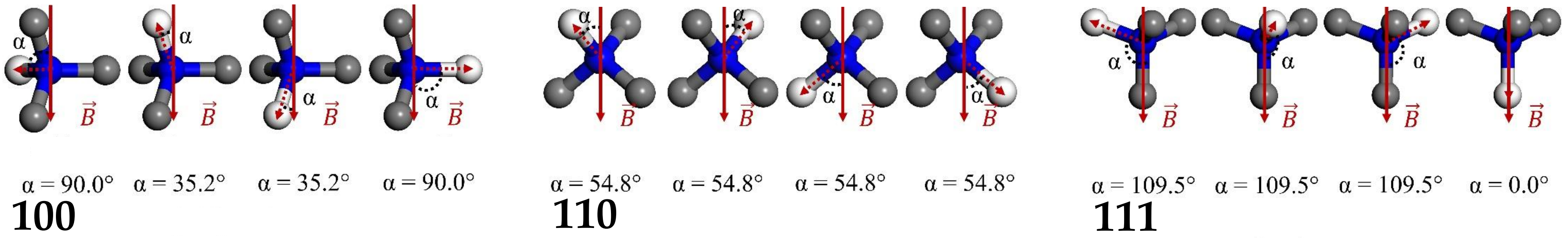
Department of Physics, ETH Zürich, 8093 Zürich, Switzerland; email: degenc@ethz.ch

Annu. Rev. Phys. Chem. 2014. 65:83–105

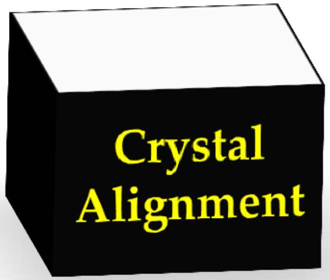
Four important issues

Crystal Alignment — NV preferential orientation.

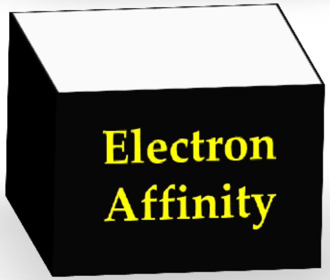
Appropriate surface orientation can maximum the photon collection efficiency.



Four important issues



— NV preferential orientation.



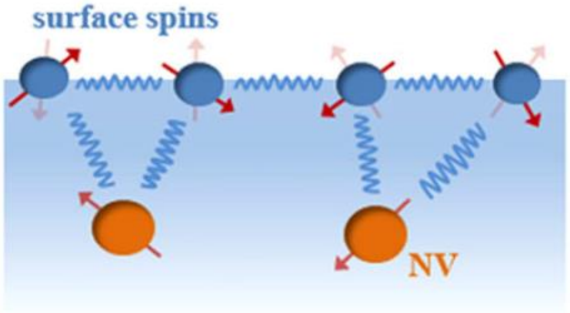
— Maintain the negatively charged state of NV.

Four important issues

Crystal Alignment — NV preferential orientation.

Electron Affinity — Maintain the negatively charged state of NV.

Surface roughness — Avoid the unwanted surface spin noise.



PRL 114, 017601 (2015)

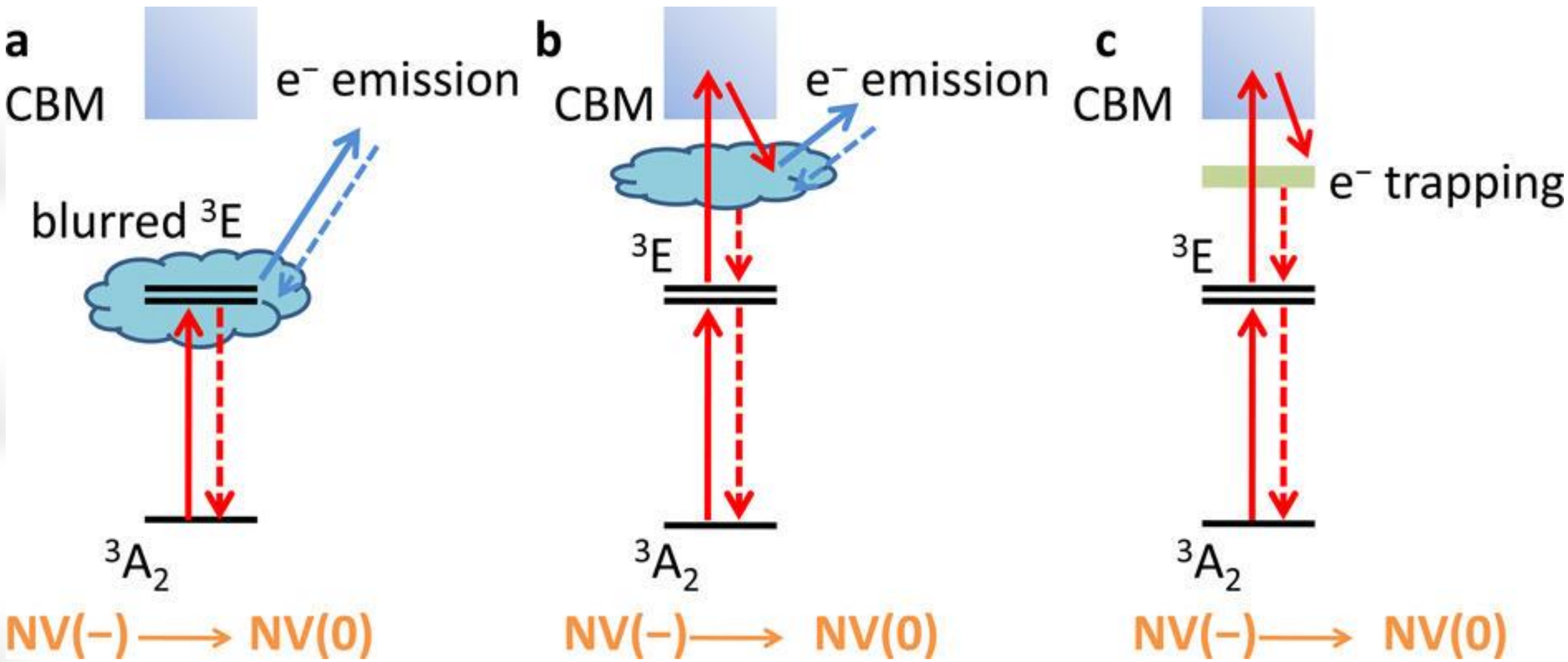
It is regardless to surface species; the origin of surface spin noise is still a mystery!

Four important issues

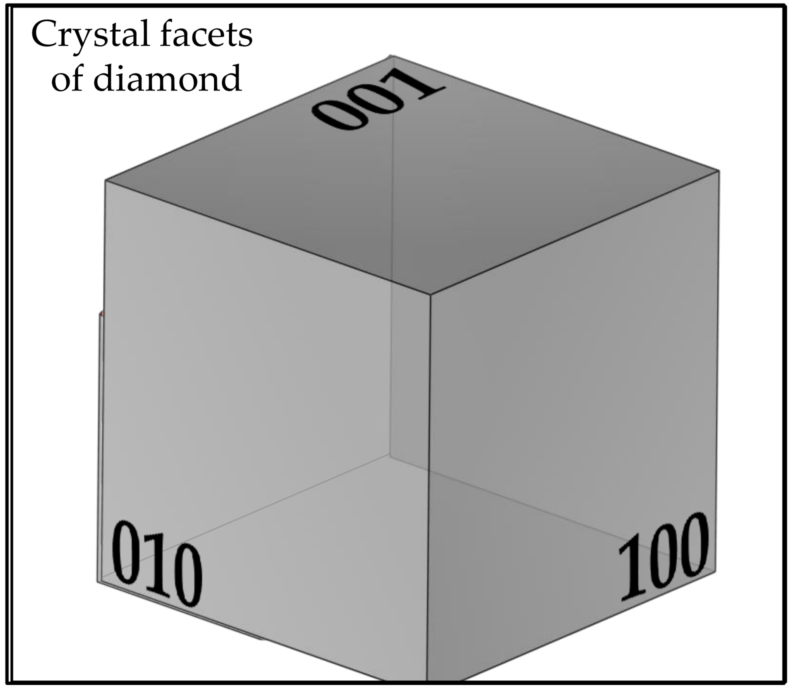
Crystal Alignment

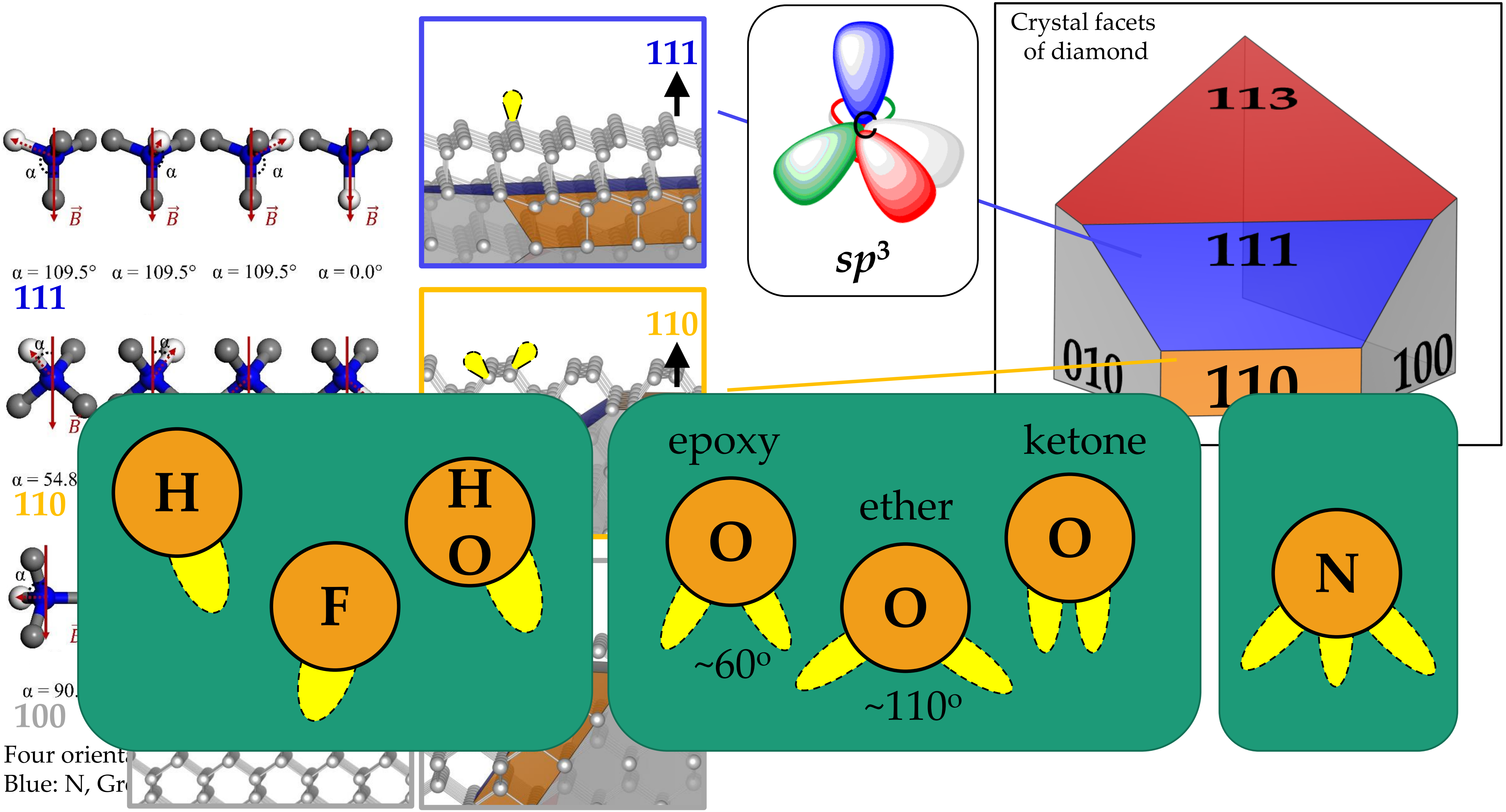
Electron Affinity

Surface roughness



Surface State —— Minimize the intrusion into the bulk bandgap.


Crystal facets
of diamond
001
010
100



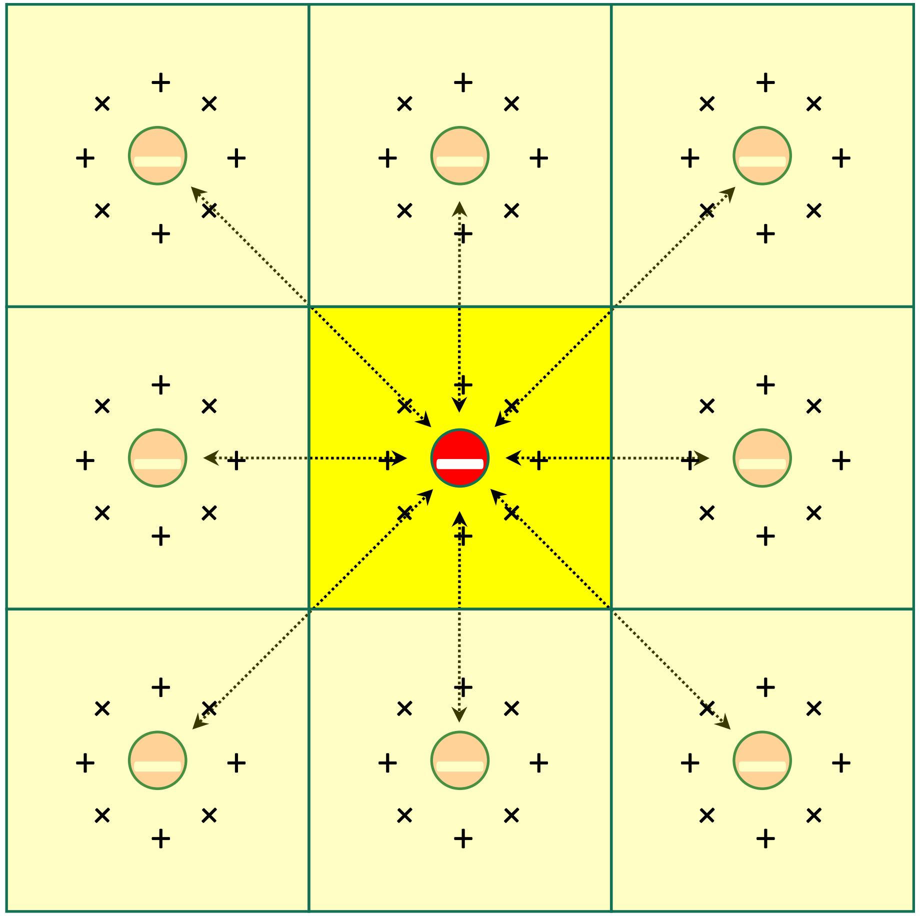
α = 109.5°
α = 109.5°
α = 109.5°
α = 0.0°
111
α = 54.8
110
α = 90.
100
Four orient
Blue: N, Gr
111
110
sp3
C
Crystal facets of diamond
113
111
010
110
100
H
F
H O
epoxy
~60°
ether
O
~110°
ketone
O
O
N

Challenges

- Underestimated bandgap of diamond:
  PBE: 4.2 eV → HSE: 5.2 eV

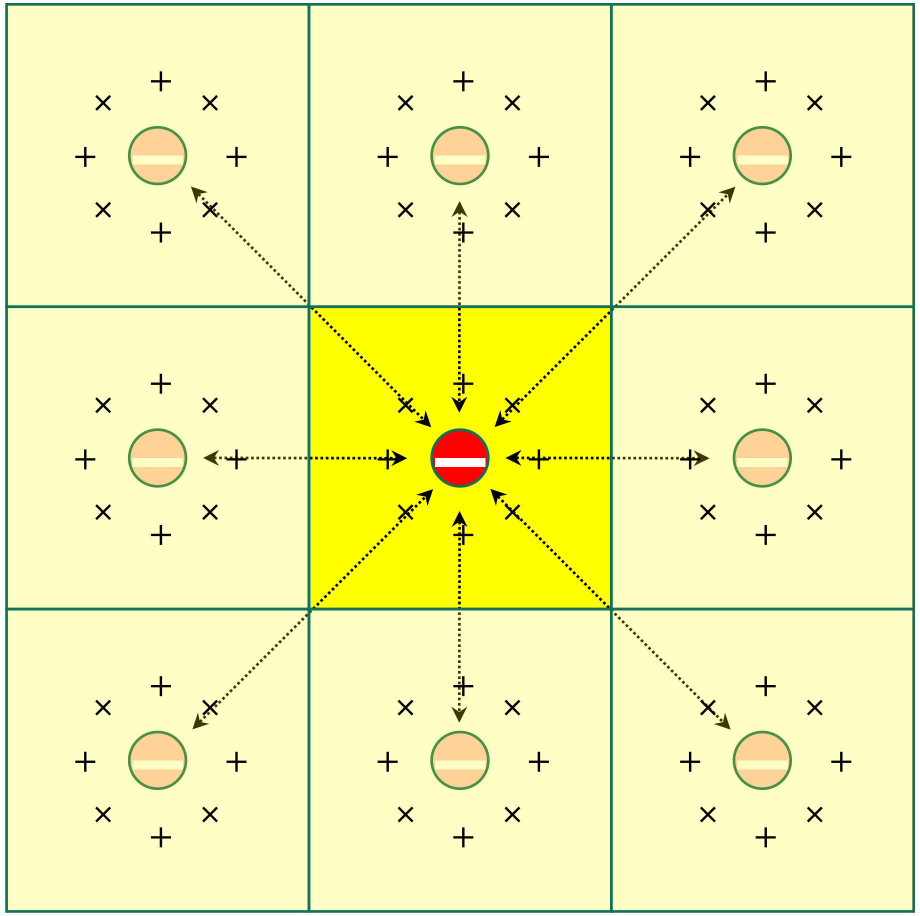
- Excitation: Constrained DFT
  [Chem. Rev. 112 (2012) 321-370]

Challenges – charged system



Spurious long-range Coulomb interactions between the localized charge and its periodic images.

Challenges



Spurious long-range Coulomb interactions between the localized charge and its periodic images.

Point charge correction: the interaction energy can be estimated from the Madelung energy of an array of point charges with neutralizing background

$$V_{PC}(q) = -\frac{\alpha q}{\varepsilon L}$$

α: Madelung constant
ε: dielectric constant
q: defect charge
L: dimension of supercell

$$E_{PC}^{corr}(q) = \frac{1}{2}\int_{\Omega}(-V_{PC})q\delta(r)dr = -\frac{q}{2}V_{PC} = \frac{\alpha q^2}{2\varepsilon L}$$

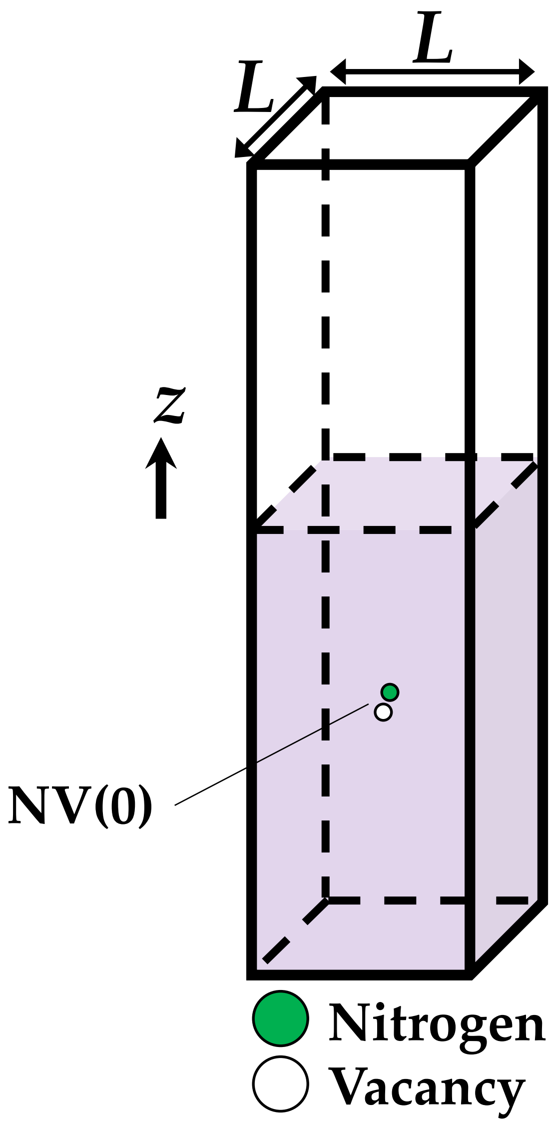
Correction schemes

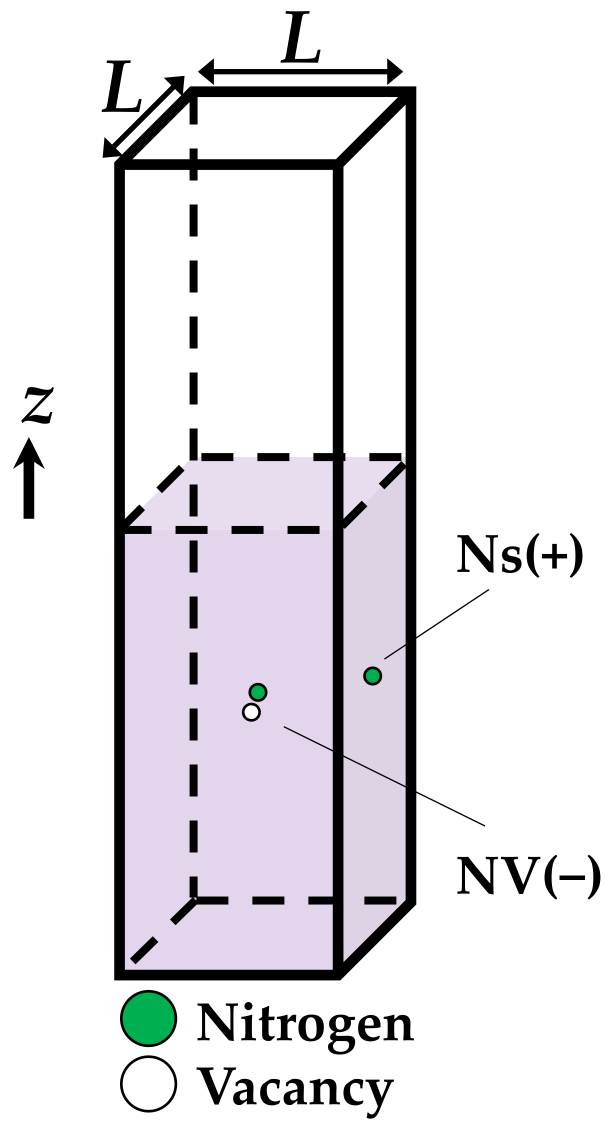
- **M. Leslie and M. J. Gillan**
  J. Phys. C: Solid State Phys. **18**, 973 (1985)
  – Madelung energy (Point-Charge correction)

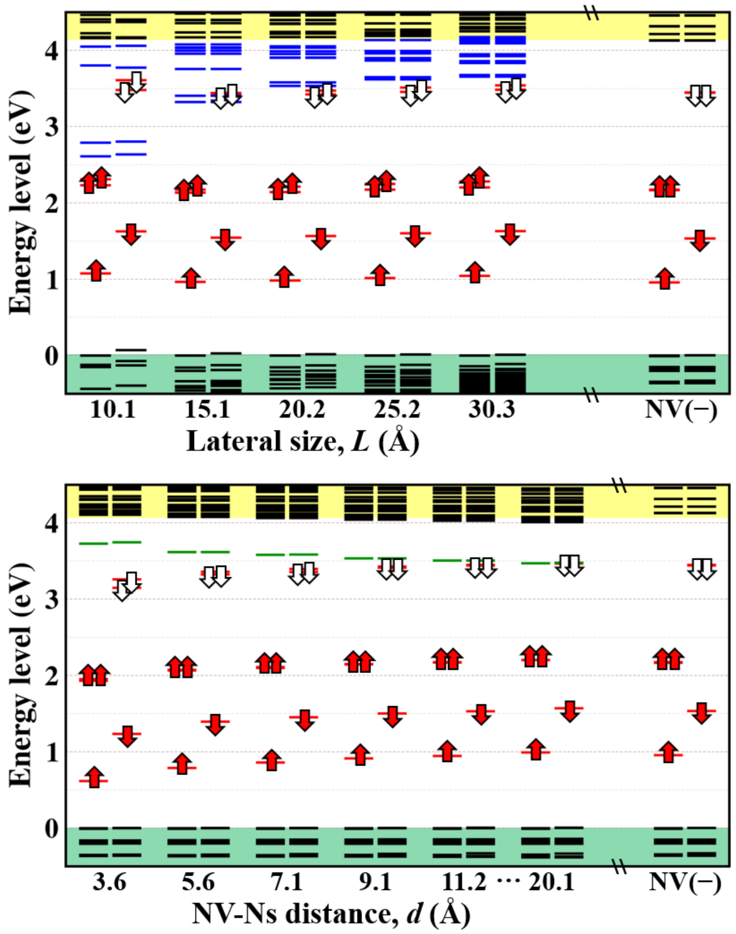
- **G. Makov and M. C. Payne (MP correction)**
  - *Phys. Rev. B* **51**, 4014 (1995)
  - C. W. M. Castleton and S. Mirbt - *Physica B* **340-342**, 407-411 (2003)
  - S. Lany and A. Zunger - *Phys. Rev. B* **78**, 235104 (2008)

- **C. Freysoldt, J. Neugebauer and C. G. Van de Walle (FNV correction)**
  - *Phys. Rev. Lett.* **102**, 016402 (2009)
  - H.-P. Komsa and A. Pasquarello - *Phys. Rev. Lett.* **110**, 095505 (2013)
  - Y. Kumagai and F. Oba - *Phys. Rev. B* **89**, 195205 (2014)

Trick

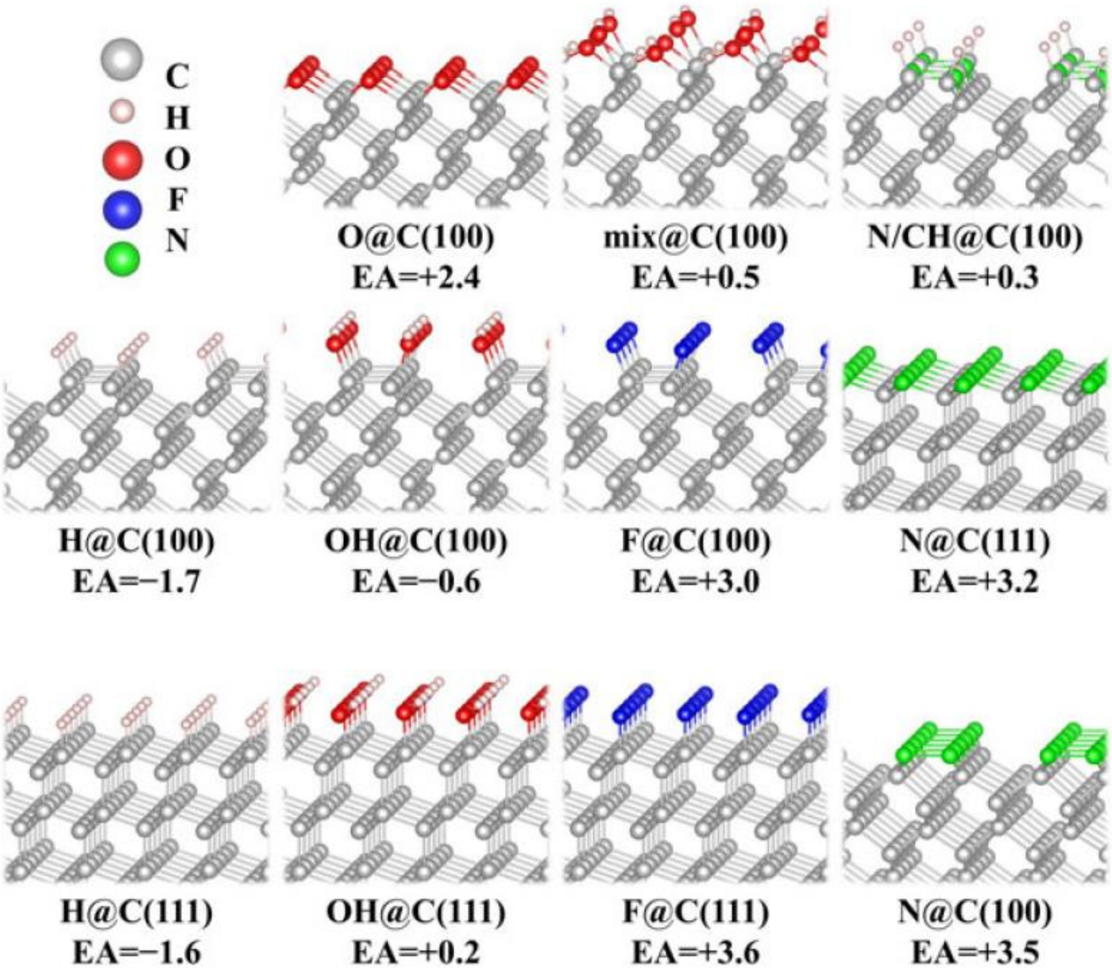






- Nano Letters **14**, 4772 (2014).
- MRS Communications **7**, 551 (2017).

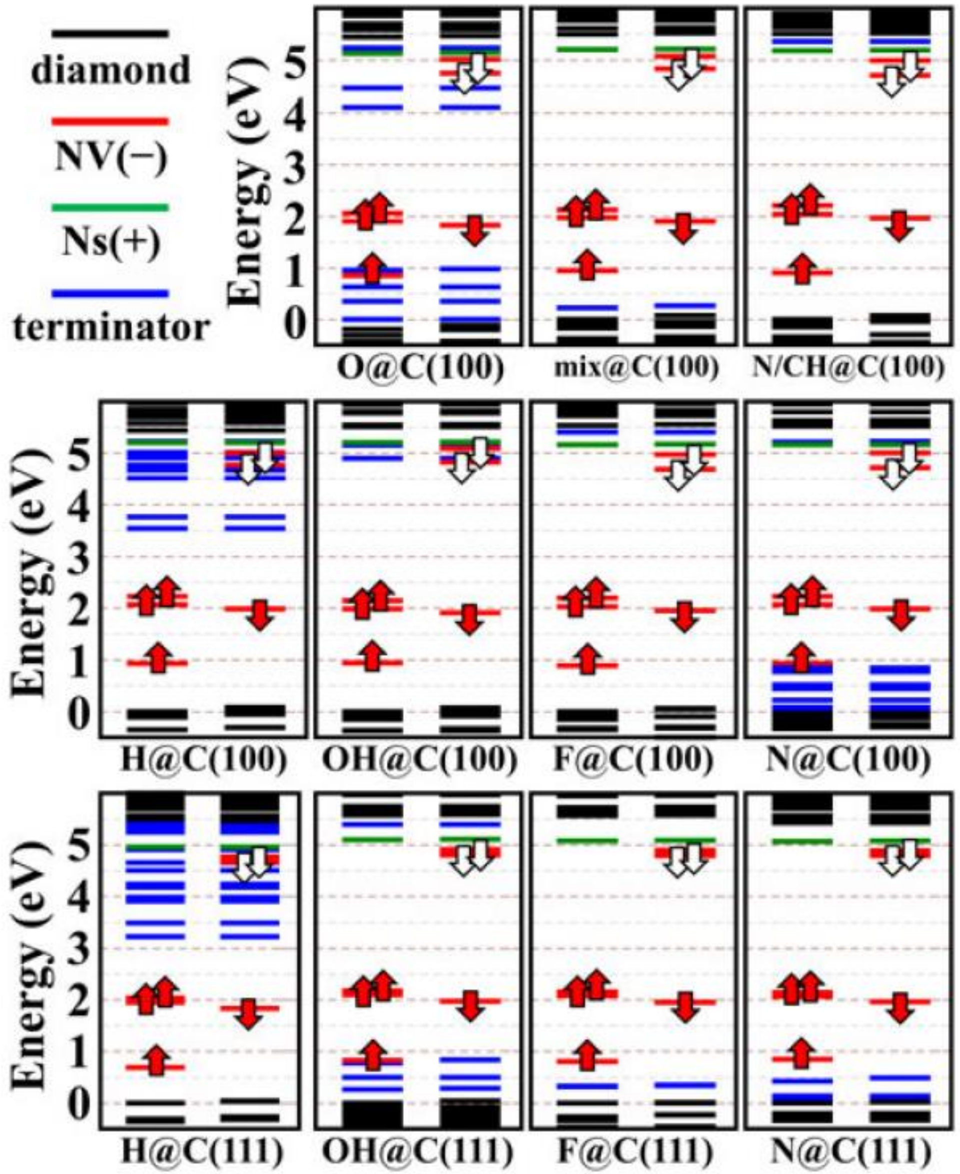
Electron affinity



- ❑ **O and F show PEA,**
  H and OH show NEA.
- ❑ **Oxidation surface is very easy, however, the oxygen induced strain will rough the surface.**
- ❑ **Fluorination might form Teflon layer.**
- ❑ **O/H/OH mixed surface is an alternative way.**
- ❑ **Nitrogen terminated diamond surface is possible.**

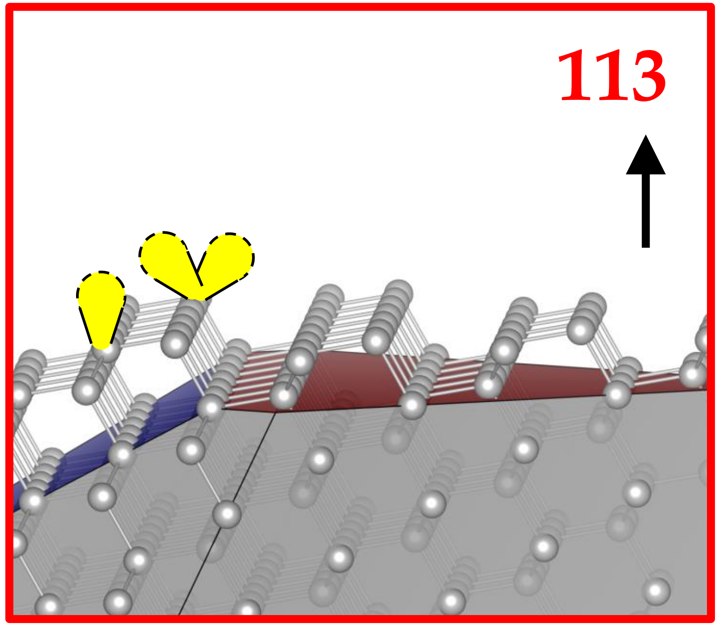
- ❖ Nano Letters **14**, 4772 (2014).
- ❖ Advanced Materials Interfaces **2**, 1500079, 1500079 (2015).
- ❖ Nano Letters **17**, 2294 (2017).
- ❖ MRS Communications **7**, 551 (2017).

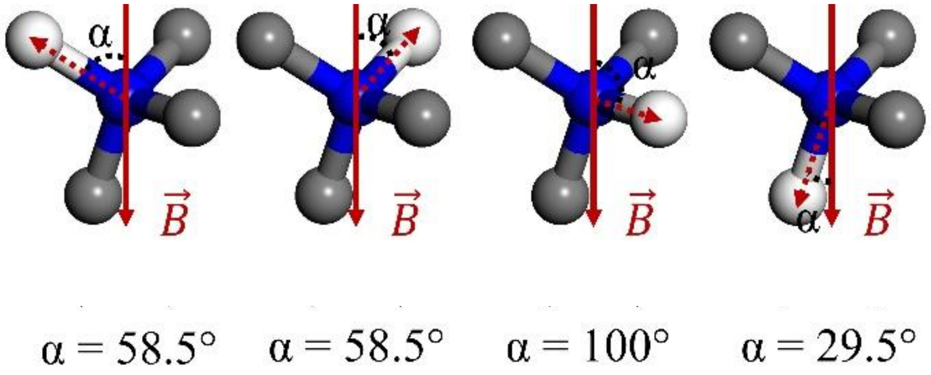
Energy levels



- ❑ Surface state intrusion occurs in H, O and OH termination cases.
- ❑ F does not show unwanted state in the bandgap.
- ❑ O/H/OH mixed surface is still pretty good.
- ❑ Nitrogen terminated diamond surface is nice.

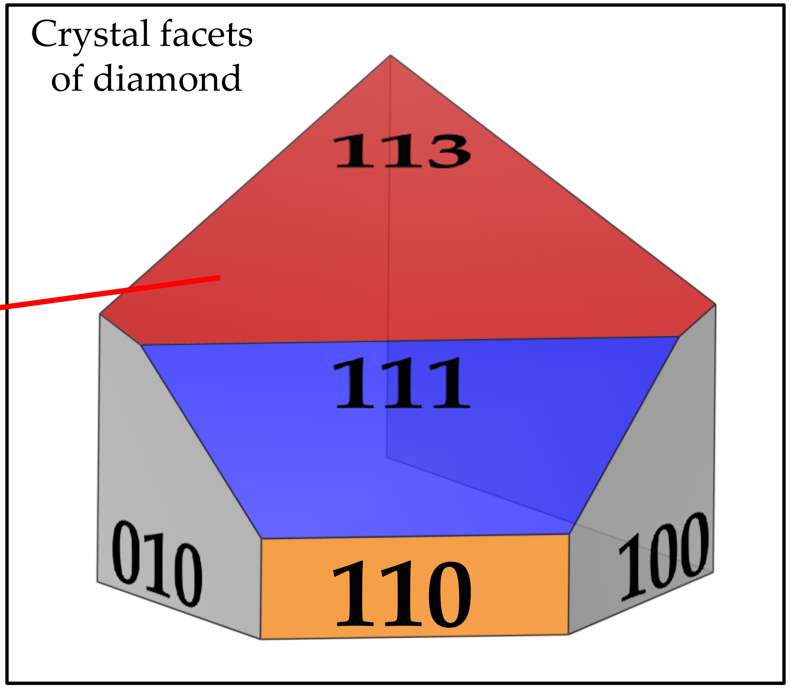
- ❖ Nano Letters **14**, 4772 (2014).
- ❖ Advanced Materials Interfaces **2**, 1500079, 1500079 (2015).
- ❖ Nano Letters **17**, 2294 (2017).
- ❖ MRS Communications **7**, 551 (2017).
- ❖ Carbon **145**, 273 (2019)

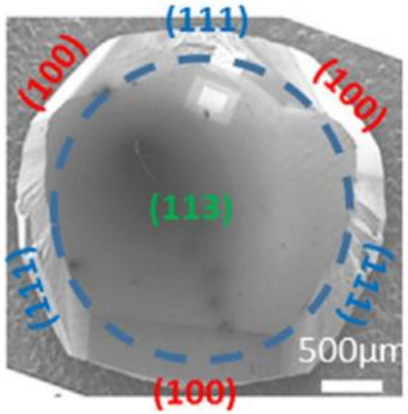




113

Four orientations of NV.
Blue: N, Grey: C, White: vacancy





M. Lesik et al. / Diamond & Related Materials 56 (2015) 47–53

SEM image of a 460 µm thick CVD film grown on a circular (113) diamond substrate.

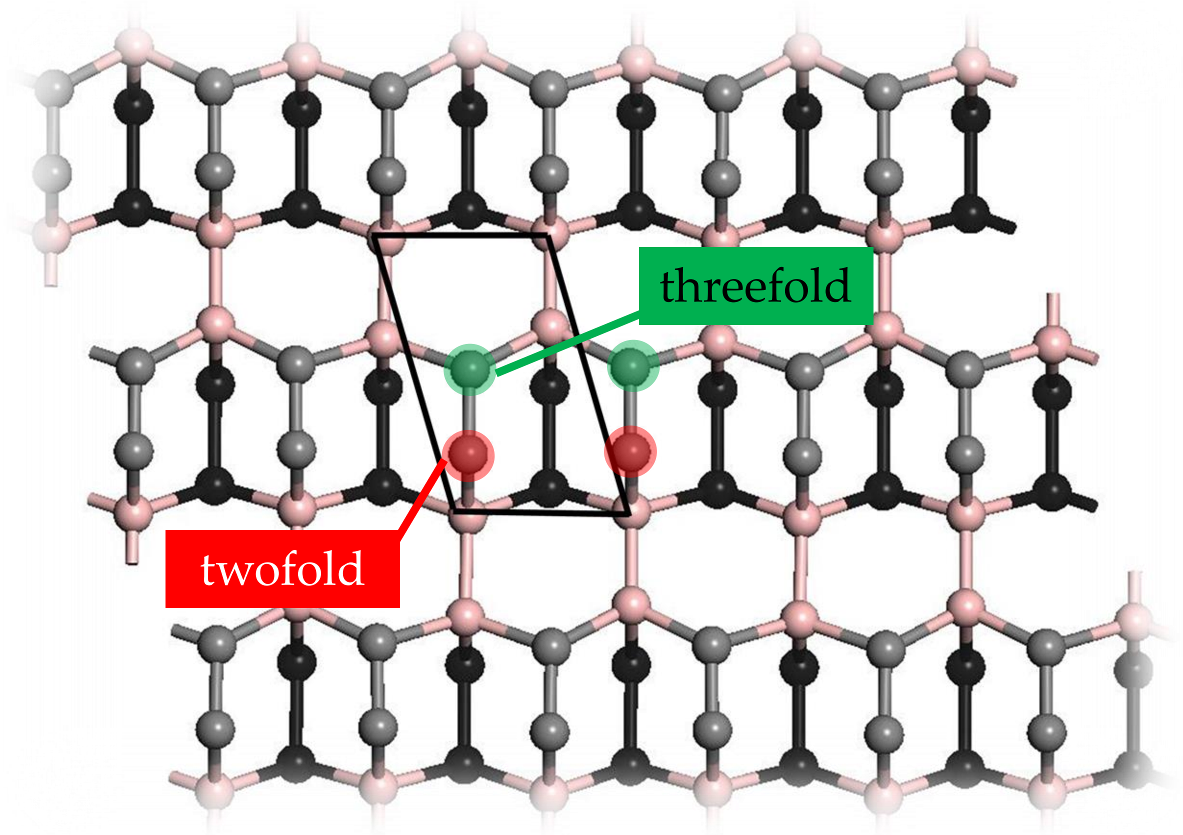
	(100)	(110)	(111)	(113)
Substrate for growth	👍 👍	👍	👎	👎
Growth condition window	👍	👍	👎	👍 👍
Growth rates	👎	👍 ×5	👎 👎	👍
Crystalline quality	👍 👍	👍	👎	👍 👍
B doping efficiency	👎	👍	👍 ×10	👍 ×5
N doping efficiency	👎	–	👍 👍	👍
NV orientation	< 50%	50%	~100%	73%
Surface terminator effects				
Surface roughness	👍	👍	👍	?
Electron affinity	H, OH, **O, F, N**	–	H, **OH, O, F, N**	H, OH, **O, F, N**
Surface state intrusion	H,OH,O, **F, N**	–	H,OH, **F, N**	H,OH, **O, F, N**

- Power Electronics Device Applications of Diamond Semiconductors. DOI: https://doi.org/10.1016/B978-0-08-102183-5.00001-7
- Diamond and Related Materials **56**, 47 (2015).
- Diamond and Related Materials **66**, 61 (2016).
- Surface Science **337**, L812 (1995).
- Applied Physics **71**, 5930 (1992).
- Crystal **7**, 166 (2017).

Our works

- Nano Letters **14**, 4772 (2014).
- Nano Letters **17**, 2294 (2017).
- Advanced Materials Interfaces **2**, 1500079, 1500079 (2015).
- MRS Communications **7**, 551 (2017).

(113) diamond: surface morphology

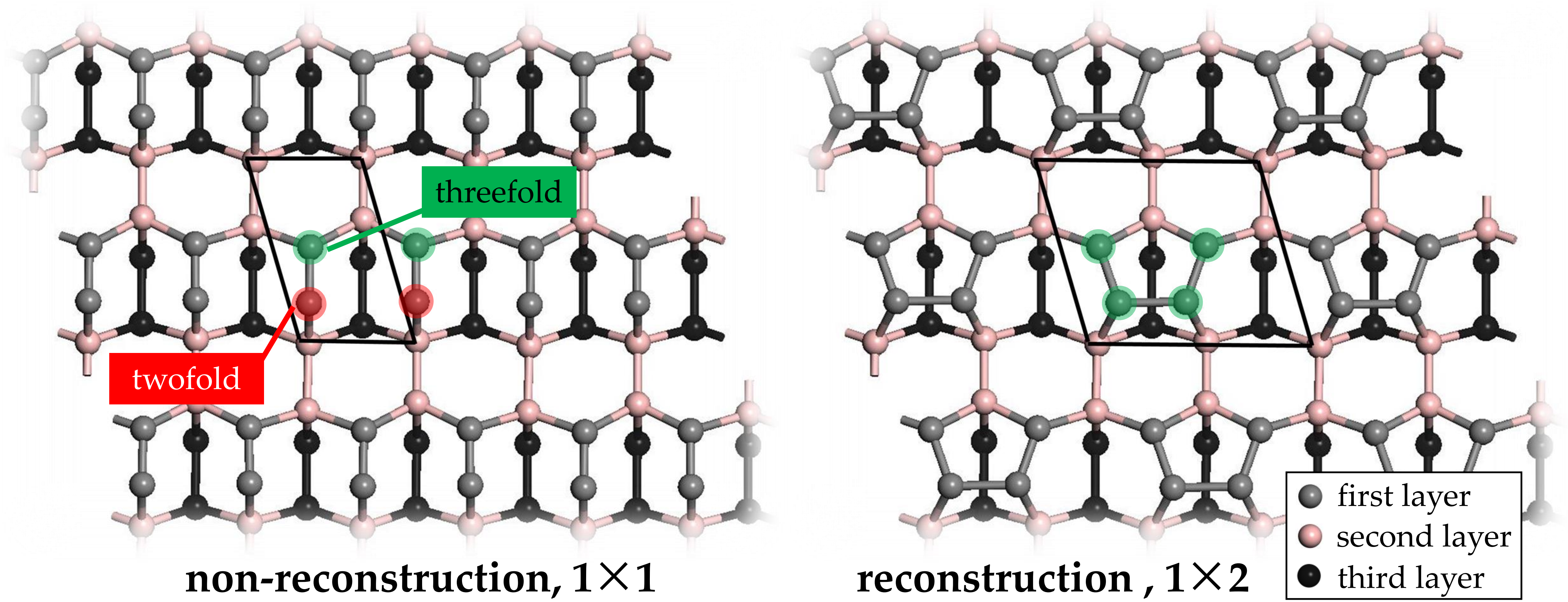


non-reconstruction, 1×1

- first layer
- second layer
- third layer

(113) diamond: surface morphology

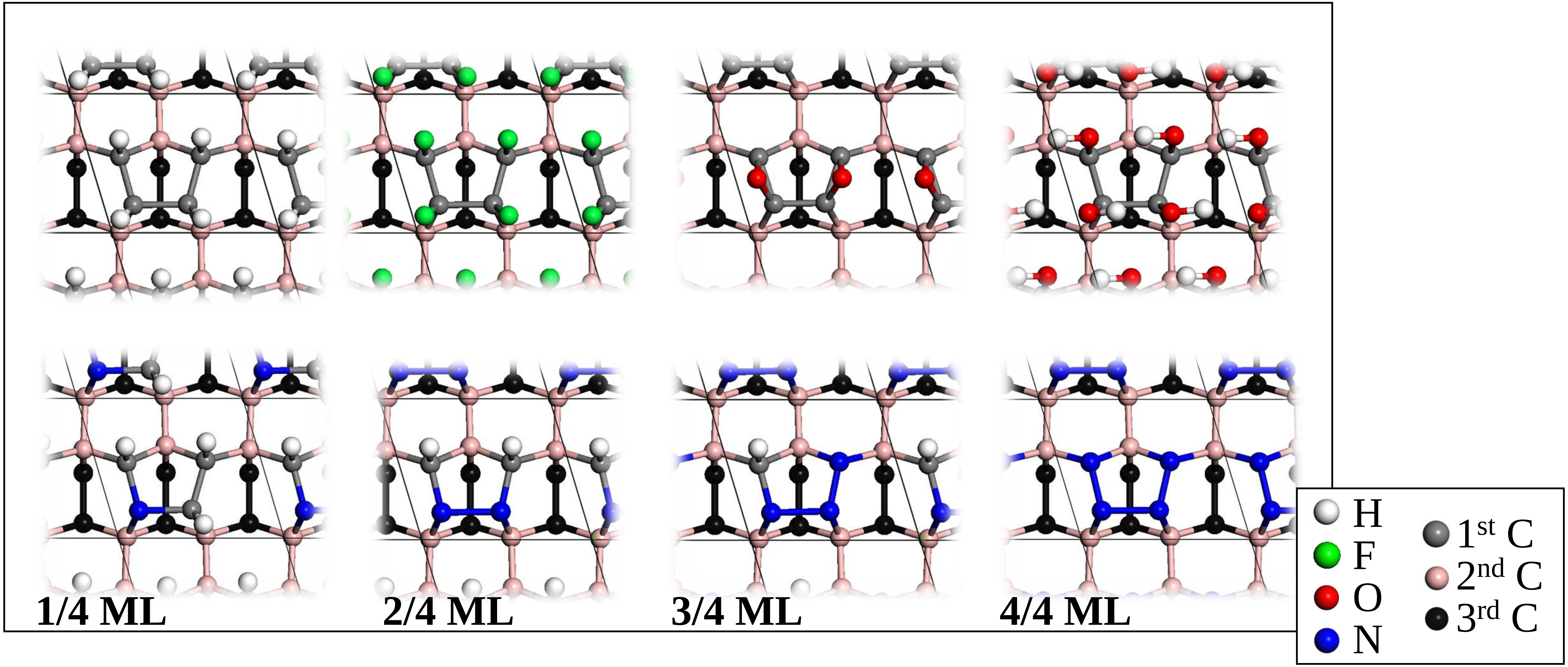
PHYSICAL REVIEW B 67, 195332 (2003)



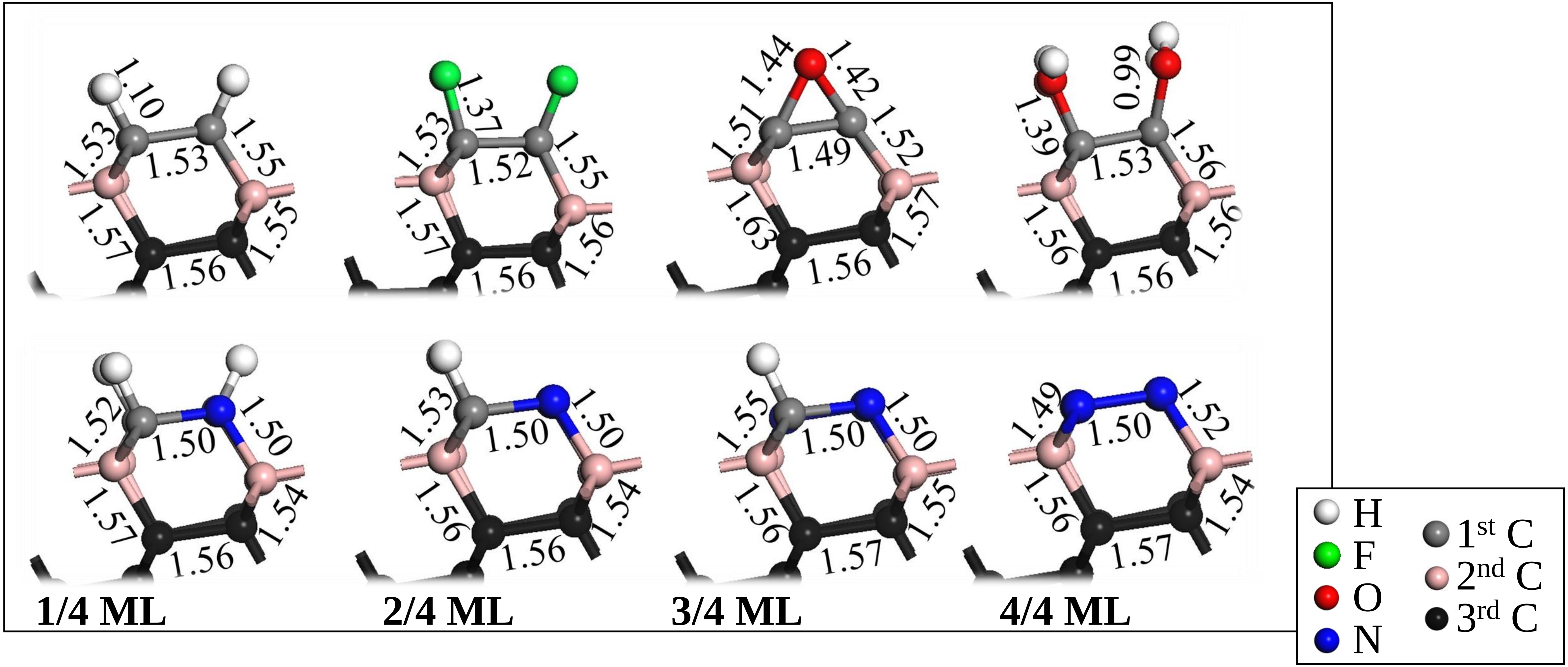
non-reconstruction, 1×1

reconstruction , 1×2

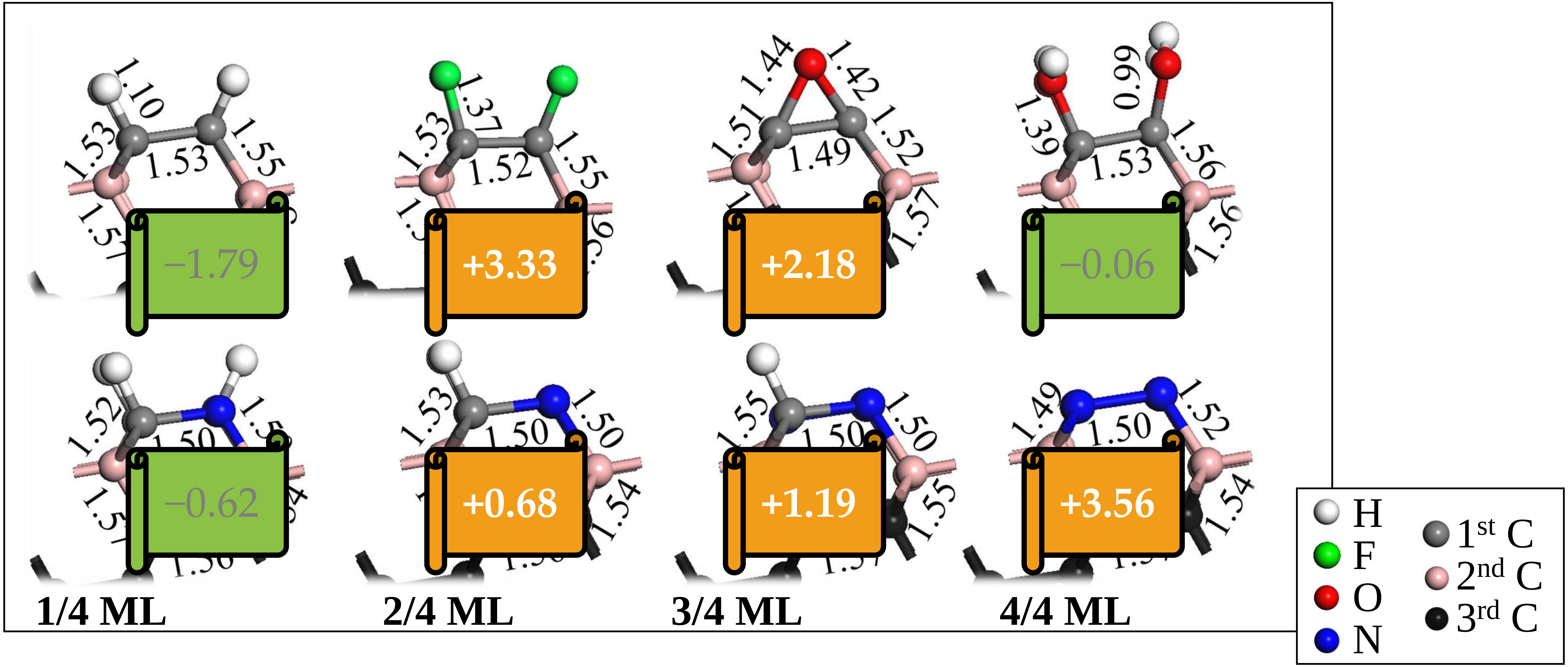
(113) diamond: Terminators, top view



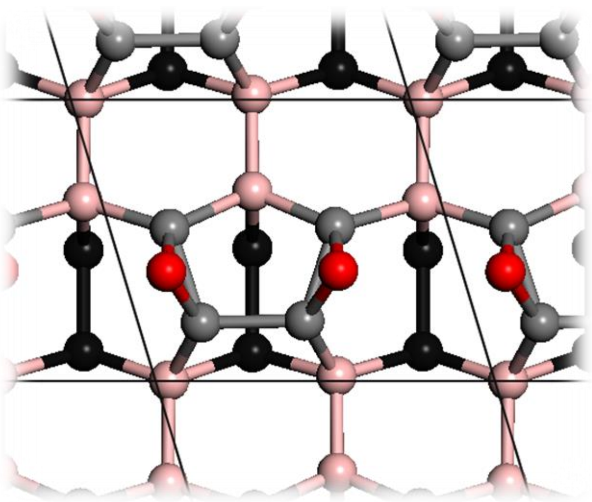
(113) diamond:
Terminators, side view

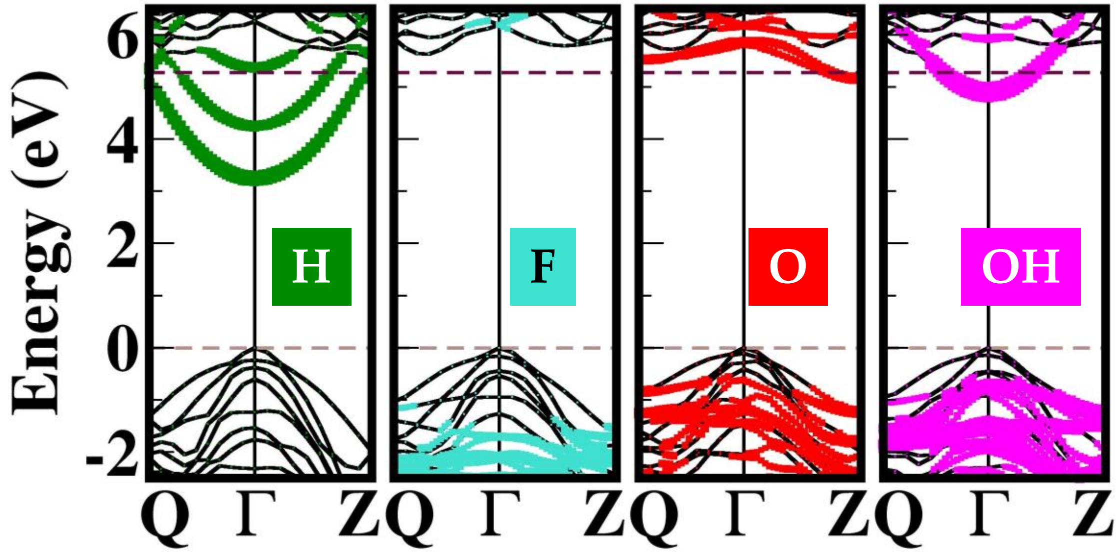


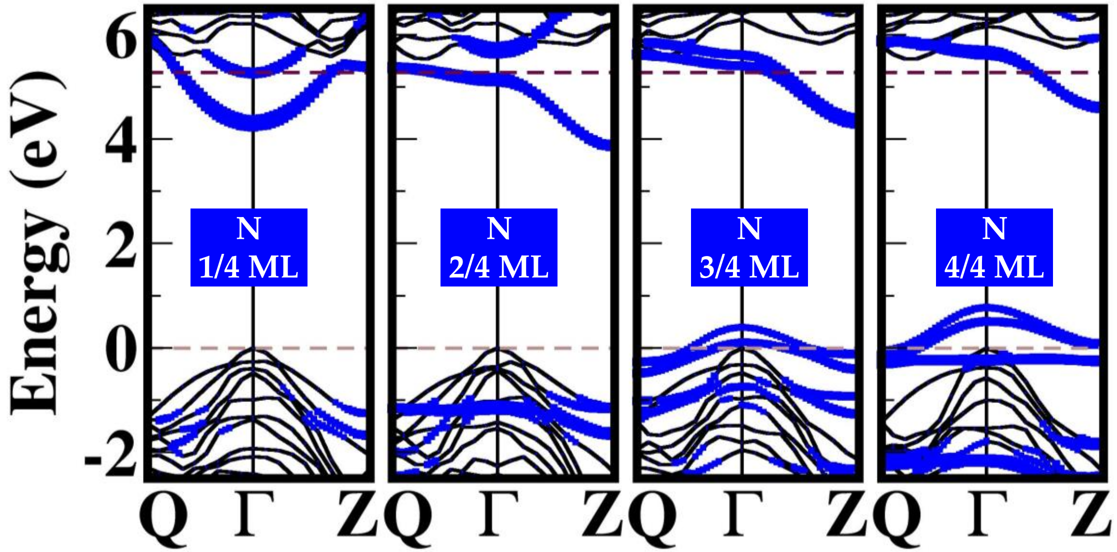
(113) diamond:
Electron affinity

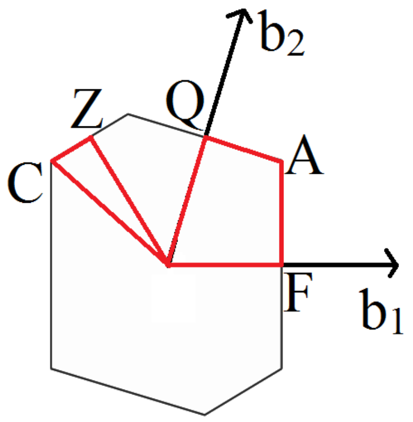


(113) diamond: Band structure



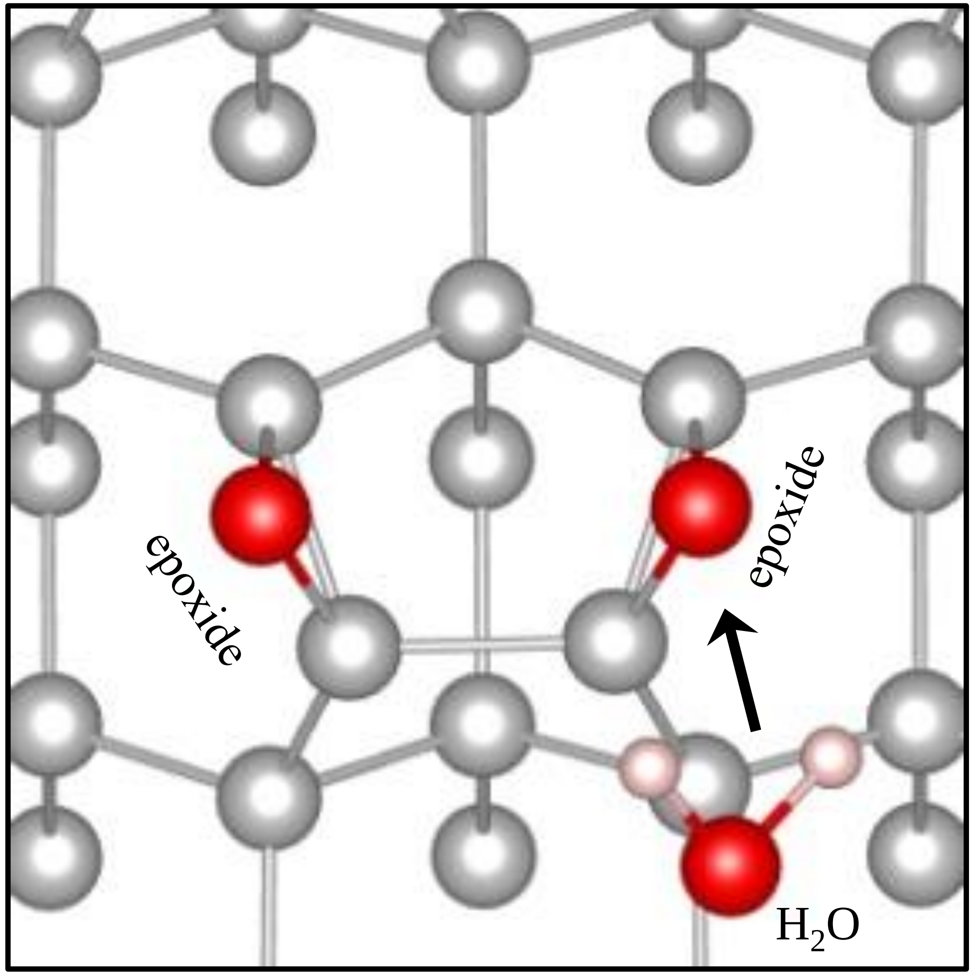




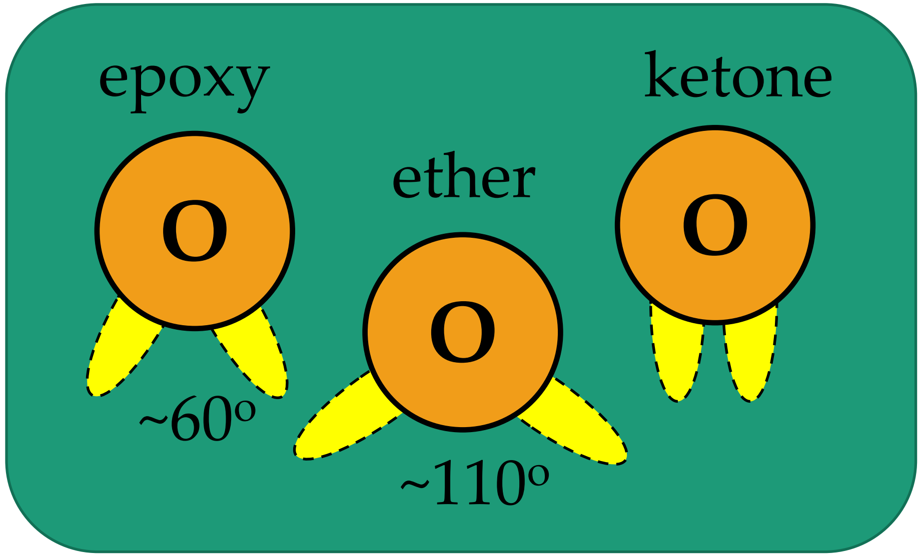


The Brillouin zone

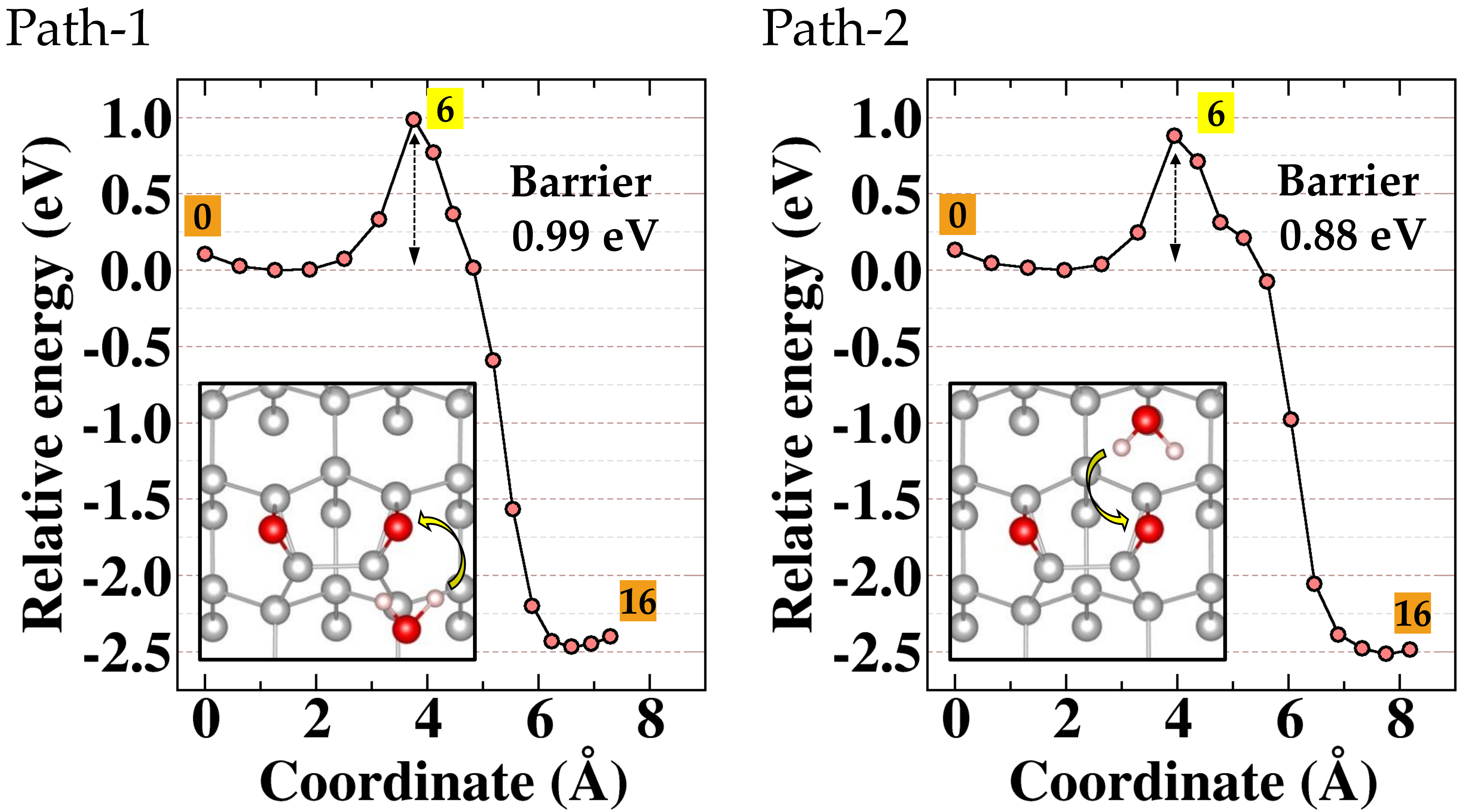
Chemical stability



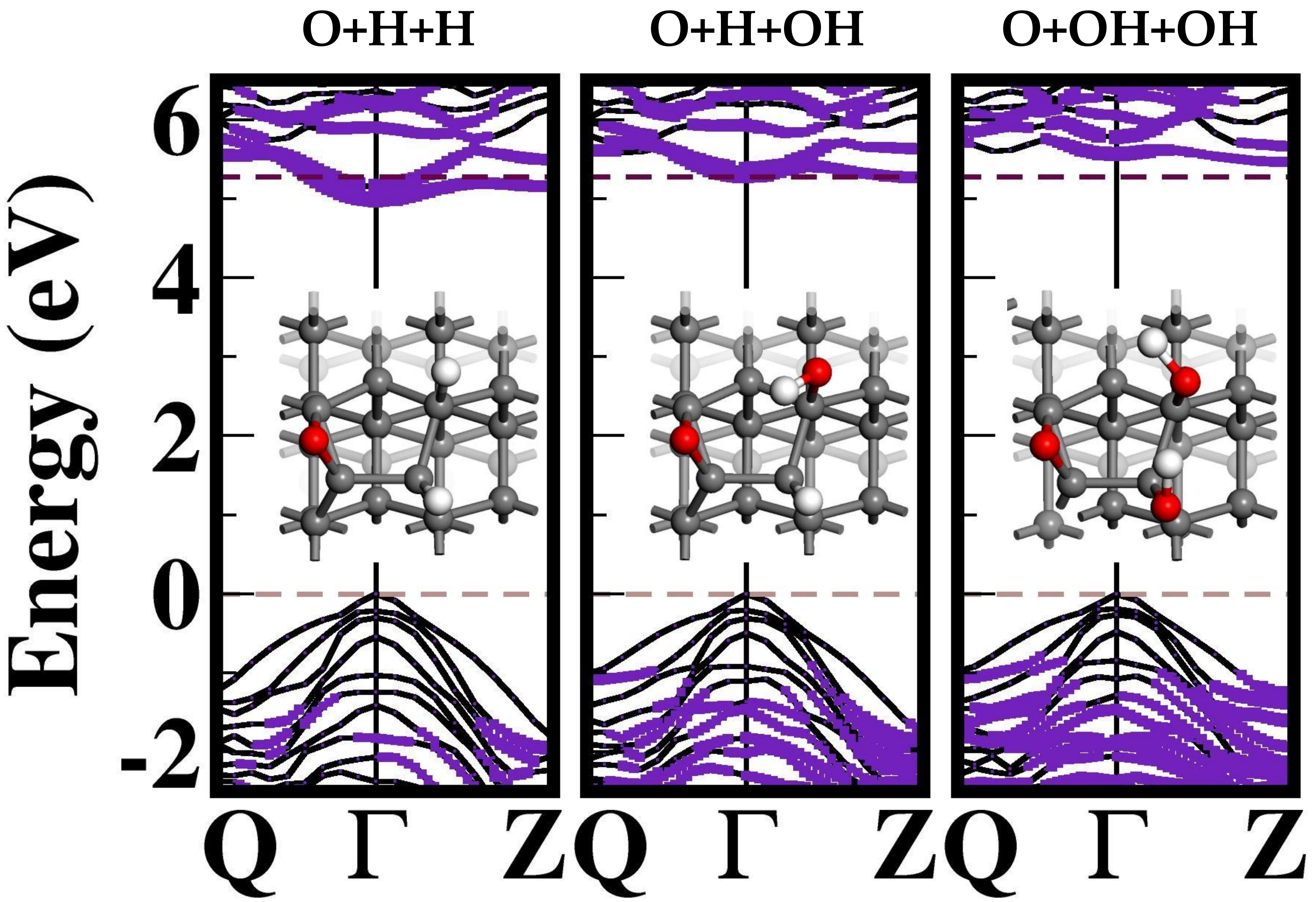
The -C-O-C- epoxide-like configuration formed on the diamond surface is stable or unstable?



Chemical stability



H/O/OH termination

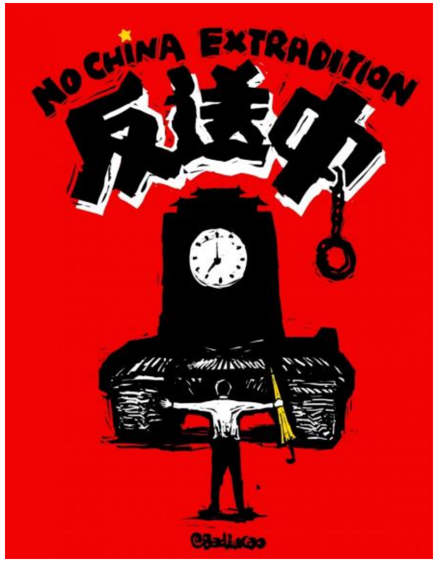


Summary

- A painless way to simulate charged system:
  NV(−) in diamond surface → NV + Ns.

- F, mixed O/H/OH, and N would be good surface termination for NV quantum sensing applications.

- Complete oxygen termination of (113) diamond creates positive electron affinity with neither strain on the surface nor in-gap levels which is supposed to be the most prospective host for NV quantum sensors.

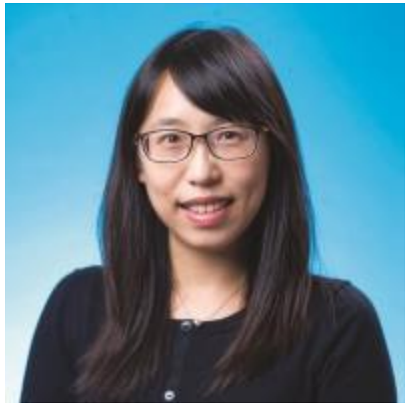


Thank you for your attention~

Ádám Gali

MAGYAR TUDOMÁNYOS AKADÉMIA 1825

WIGNER



Alice Hu

Song Li

CityU
香港城市大學
City University of Hong Kong

Conclusion

- In general, the physical and chemical properties of (113) are better than other facets.

	(100)	(110)	(111)	(113)
Substrate for growth	👍 👍	👍	👎	👎
Growth condition window	👍	👍	👎	👍 👍
Growth rates	👎	👍 ×5	👎 👎	👍
Crystalline quality	👍 👍	👍	👎	👍 👍
B doping efficiency	👎	👍	👍 ×10	👍 ×5
N doping efficiency	👎	–	👍 👍	👍
NV orientation	< 50%	50%	~100%	73%
Surface terminator effects				
Surface roughness	👍	👍	👍	**?**
Electron affinity	H, OH, **O, F, N**	–	H, **OH, O, F, N**	H, OH, **O, F, N**
Surface state intrusion	H,OH,O, **F, N**	–	H,OH, **F, N**	H,OH, **O, F, N**

- ***Oxygenated*** (113) could be a promising candidate surface for NV quantum sensing in diamond.

	(100)	(110)	(111)
Substrate for growth	👍 👍	👍	👎
Growth condition window	👍	👍	👎
Growth rates	👎	👍 ×5	👎 👎
Crystalline quality	👍 👍	👍	👎
B doping efficiency	👎	👍	👍 ×10
N doping efficiency	👎	–	👍 👍
NV orientation	< 50%	50%	~100%
Surface terminator effects			
Surface roughness	👍	👍	👍
Electron affinity	H, OH, **O, F, N**	–	H, **OH, O, F, N**
Surface state intrusion	H,OH,O, **F, N**	–	H,OH, **F, N**

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- MRS Communications **7**, 551 (2017).

Blue: N, Grey: C, White: vacancy

	(100)	(110)	(111)	(113)
Substrate for growth	👍 👍	👍	👎	👎
Growth condition window	👍	👍	👎	👍 👍
Growth rates	👎	👍 ×5	👎 👎	👍
Crystalline quality	👍 👍	👍	👎	👍 👍
B doping efficiency	👎	👍	👍 ×10	👍 ×5
N doping efficiency	👎	–	👍 👍	👍
NV orientation	< 50%	50%	~100%	73%
Surface terminator effects				
Surface roughness	👍	👍	👍	👎
Electron affinity	H, OH, **O, F, N**	–	H, **OH, O, F, N**	**?**
Surface state intrusion	H,OH,O, **F, N**	–	H,OH, **F, N**	**?**

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