50 years of the Institute of High Pressure Physics Polish Academy of Sciences

Highlights in III-V semiconductors, THz physics and nanomaterials

Anniversary Symposium „Unipress 50”

Charge related phenomena at semiconductor surfaces

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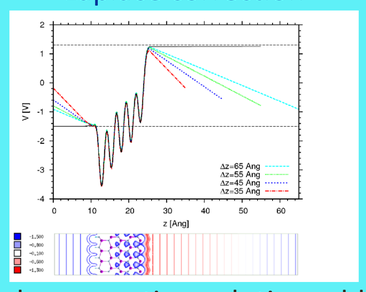
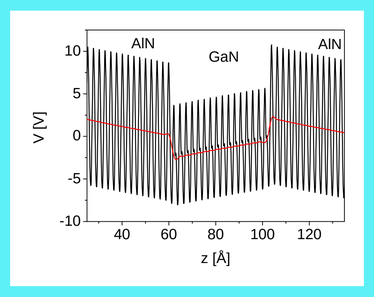
New methodology – *ab initio* calculations (SIESTA & VASP)

Laplace correction



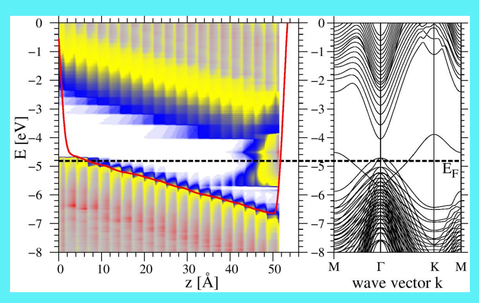
- Laplace equation solution added to Poisson solution equation
- Periodic boundary condition
- No dipole layer in the empty space

Potential averaging



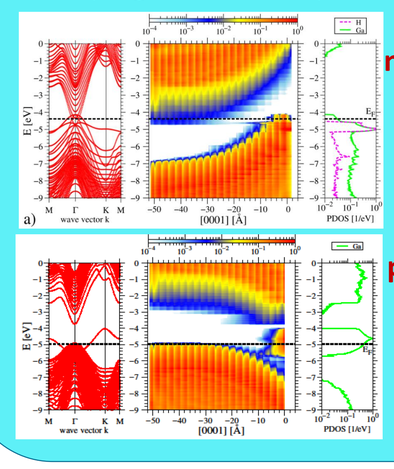
- In-plane and c-axis adjacent averaging
- Smoothed potential profiles
- Charges & dipoles are obtained

Real space band visualization



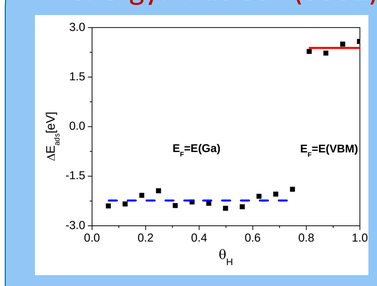
- Fields in the slabs
- Charged surface states
- Fermi level pinning

Doping- Fermi level pinning



New results

Charge contribution to adsorption energy: H at GaN(0001) surface



Adsorption energy jump at

$$\theta_H = \frac{3}{4} ML$$

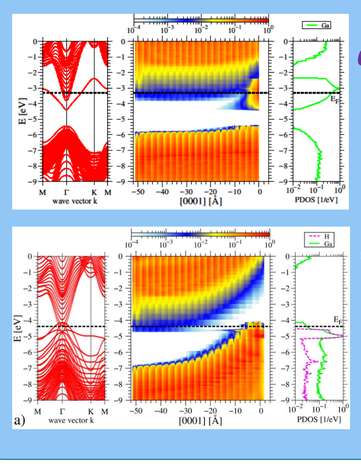
No electrons in Ga broken bond state

α - Ga broken bond – ¾ electron

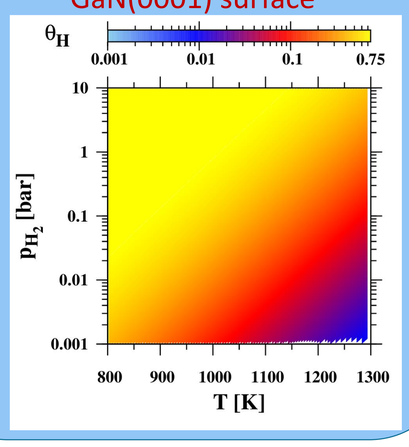
β - H – 1 electron (+ ¾ electron from Ga)

$$\frac{3}{4}\alpha + \left(1+\frac{3}{4}\right)\beta = 2\beta + 0\alpha \qquad \beta = 3\alpha = \frac{3}{4}$$

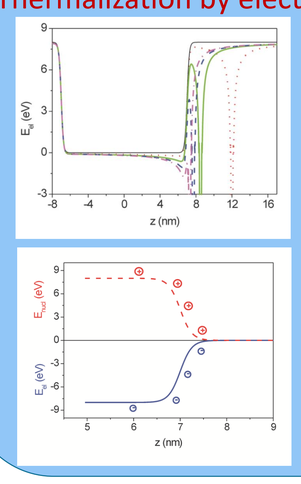
Fermi level pinning



Phase diagrams – H at GaN(0001) surface



Thermalization by electron tunneling

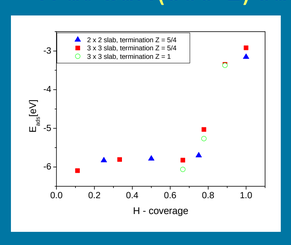


Combined potential profile

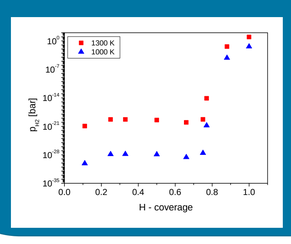
Kinetic energy dissipation after tunneling

Semiconductor surfaces & adsorbates

H at GaN(000-1) surface

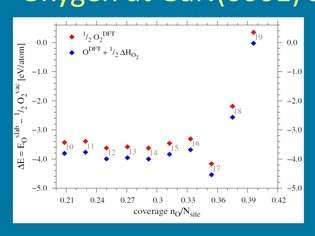


Adsorption energy

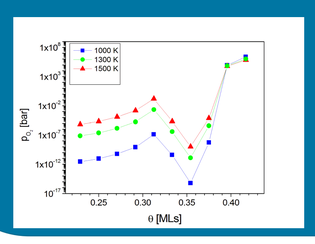


Pressure – coverage diagram

Oxygen at GaN(0001) surface

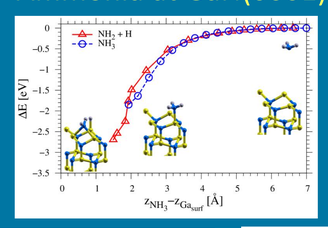


Adsorption energy

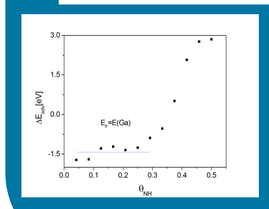


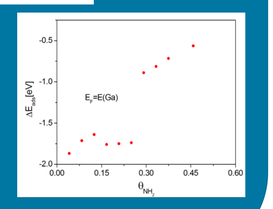
Pressure – coverage diagram

Ammonia at GaN(0001) surface



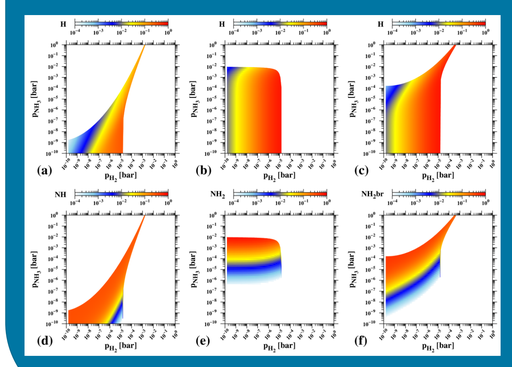
Adsorption path





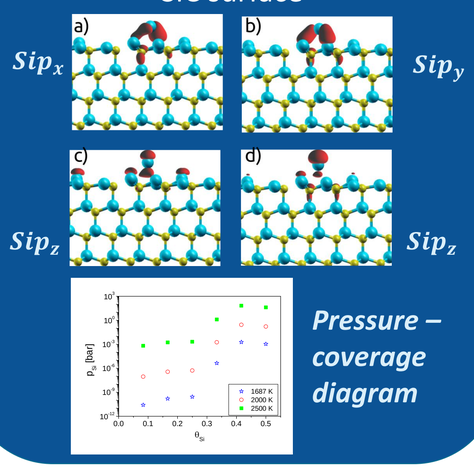
Ammonia at GaN(0001) surface

H and N related radicals coverage



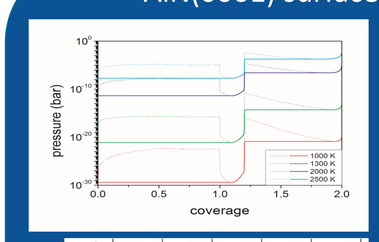
Semiconductor surfaces & adsorbates

SiC surface

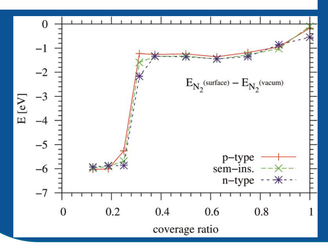


Pressure – coverage diagram

AlN(0001) surface

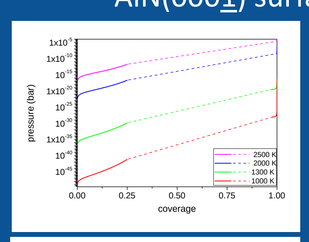


Aluminum

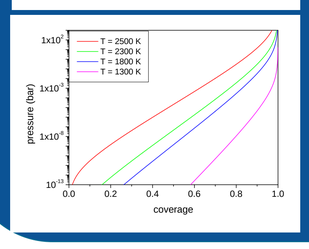


Nitrogen

AlN(000$\underline{1}$) surface



Aluminum



Nitrogen

Summary

- Laplace correction for slab simulations
- Averaging procedures for *ab initio data*
- Doping in surface slab simulations
- Charge transfer contribution to adsorption energy
- Adsorbate thermalization model
- Thermal contribution to free energy of the adsorbate
- Pressure-coverage diagrams for number of semiconductor surfaces

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