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1990-1994: Kossuth Lajos Gymnasium, Cegléd, Hungary
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1996-2001: University of Technology and Economics Budapest, Hungary
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2000: Erasmus scholarship in Paderborn [*]

2001: Master degree in Atomic Physics Department :

Master thesis: Hydrogen study in III-Nitride semiconductor
by quantumchemical calculations.[**]

01.08.2001: member of the DIODE EU-project.

[*] Band structure and optical properties of germanium sheet polymers

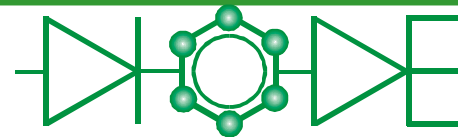
Z. Hajnal, G. Vogg, Lex J.-P. Meyer, B. Szucs, M. S. Brandt, Th. Frauenheim. Phys. Rev. B. **64** 033311 (2001)

[**] The physics and chemistry of hydrogen in the vacancies of semiconductors

B. Szucs, Á. Gali, Z. Hajnal, P. Deák, C. G. Van de Walle in print.



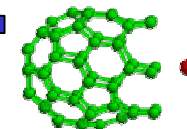
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Paderborn*

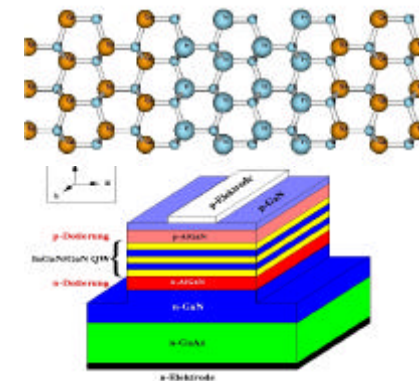
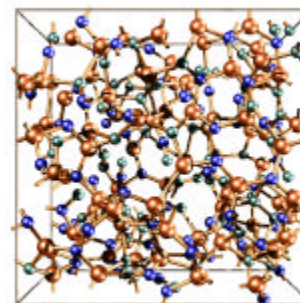
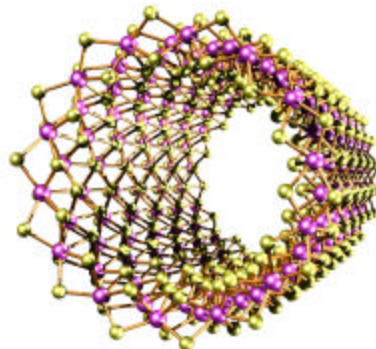
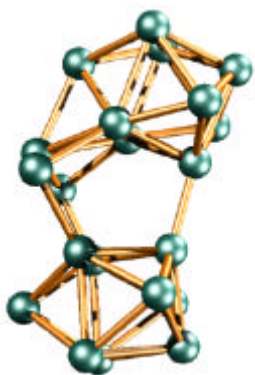


PTCDA on S:GaAs(100)



Bernadett Szucs, Zoltán Hajnal

Thomas Frauenheim group, University of Paderborn

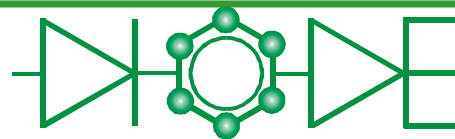


Responsibilities: Fundamentals of organic/inorganic heterojunction by approximate density functional theory.

- Contents:**
- Method (DFTB)
 - PTCDA molecular crystal
 - S:GaAs(100)
 - Single PTCDA molecule on S:GaAs
 - Conclusion



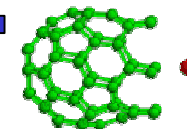
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Method



SCC-DFTB [1]: 2.order-expansion of Kohn-Sham energy functional

$$\mathbf{E}[\mathbf{n}_0 + d\mathbf{n}] = \sum_i^{\text{occ}} \mathbf{n}_i \langle Y_i | \hat{\mathbf{H}}_0 | Y_i \rangle + E_{\text{rep}}[\mathbf{n}_0] + E(d\mathbf{n}^2)$$
$$E[d\mathbf{n}^2] = \frac{1}{2} \sum_{IJ} Dq_I Dq_J g_{IJ}$$

Y_i – LCAO minimal basis representation Dq – Mulliken-charge approximation

Hybrid SCC-DFTB [2]: additional empirical potential to describe the van der Waals and weak intermolecular hydrogen bonding.

$$\tilde{E}_{\text{rep}}[\mathbf{n}_0] = E_{\text{rep}}[\mathbf{n}_0] + E_{\text{dis}} \quad E_{\text{dis}} = \sum_{IJ} \frac{(\mathbf{I}_I a_I)(\mathbf{I}_J a_J)}{(\mathbf{I}_I + \mathbf{I}_J) \mathbf{R}_{IJ}^6}$$

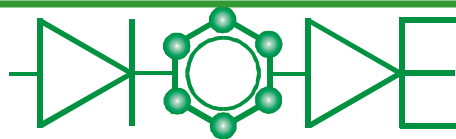
Description of van der Waals interaction is also a deficiency of the DFT.

[1] M. Elstner et al. Phys. Rev. B **58** 7260 (1998)

[2] M. Elstner and P. Hobza, J. Chem. Phys. **114** 5149 (2001)



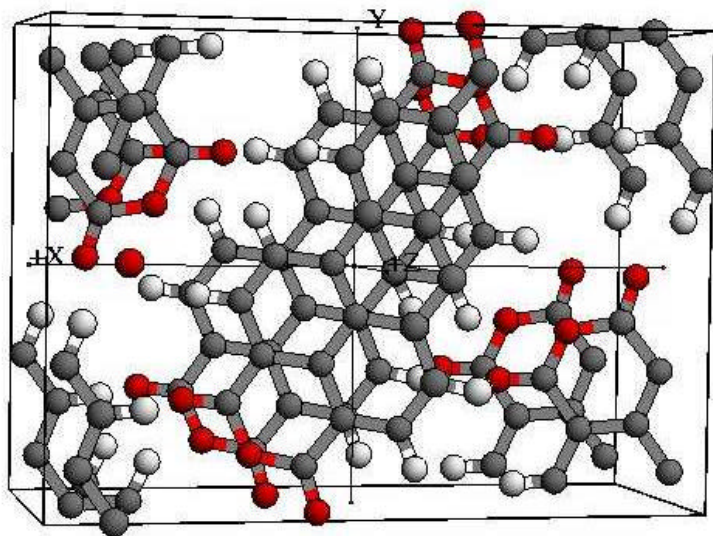
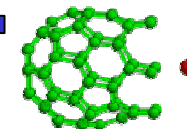
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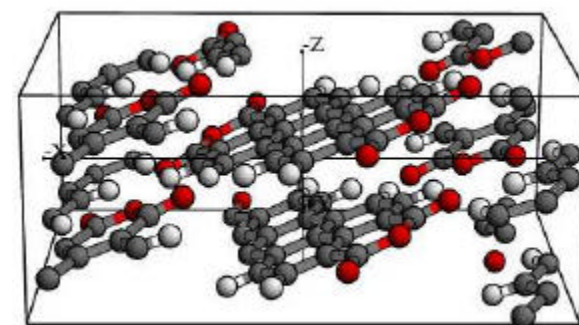


PTCDA molecular crystal

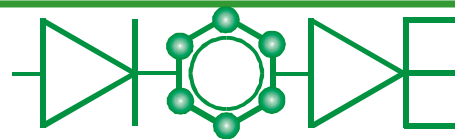
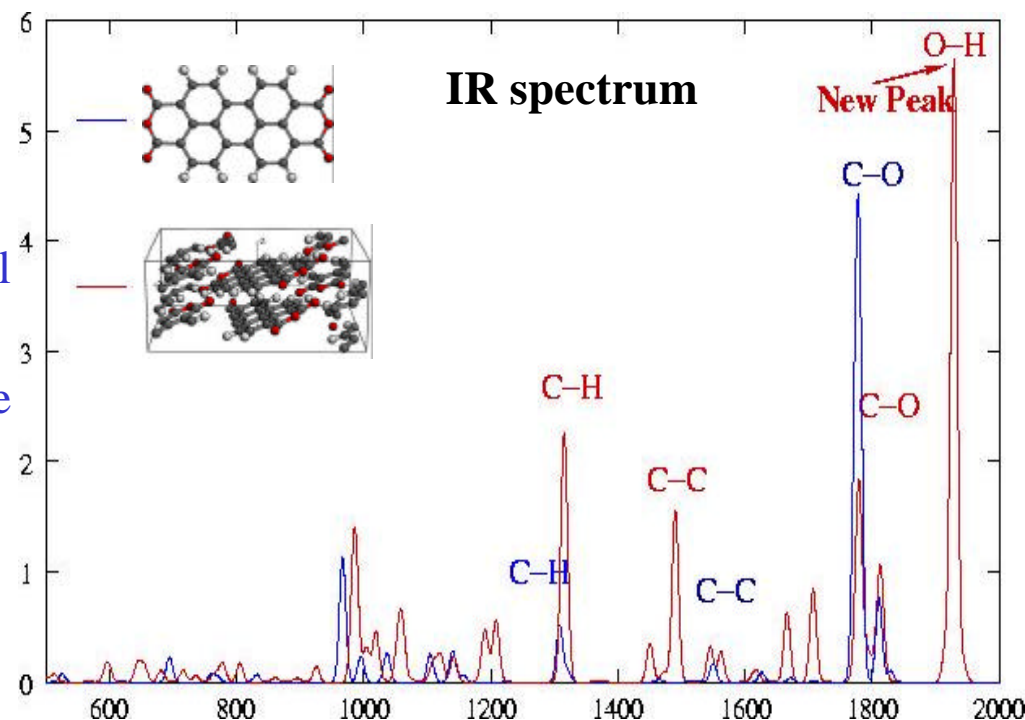


- minimization of the energy by cell optimization, θ was fixed
- $a = 17.34 \text{ \AA}$, $b = 11.96 \text{ \AA}$,
 $c = 3.72 \text{ \AA}$, $\theta = 98.8^\circ$ experimental

$a = 16.84 \text{ \AA}$
 $b = 12.68 \text{ \AA}$
 $c = 3.69 \text{ \AA}$
 $\theta = 98.8^\circ$

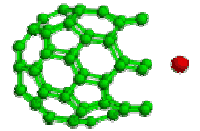


- Compared the IR spectrum of the molecular crystal and one single molecule.
- **New Peak** at 1930 1/cm : intermolecular O-H mode
- **C-C, C-H enhanced**: the dimer PTCDA move together.
- **C-O decrease**: in the dimer contrary motion
- **Binding energy** between the PTCDA: **1.65 eV**

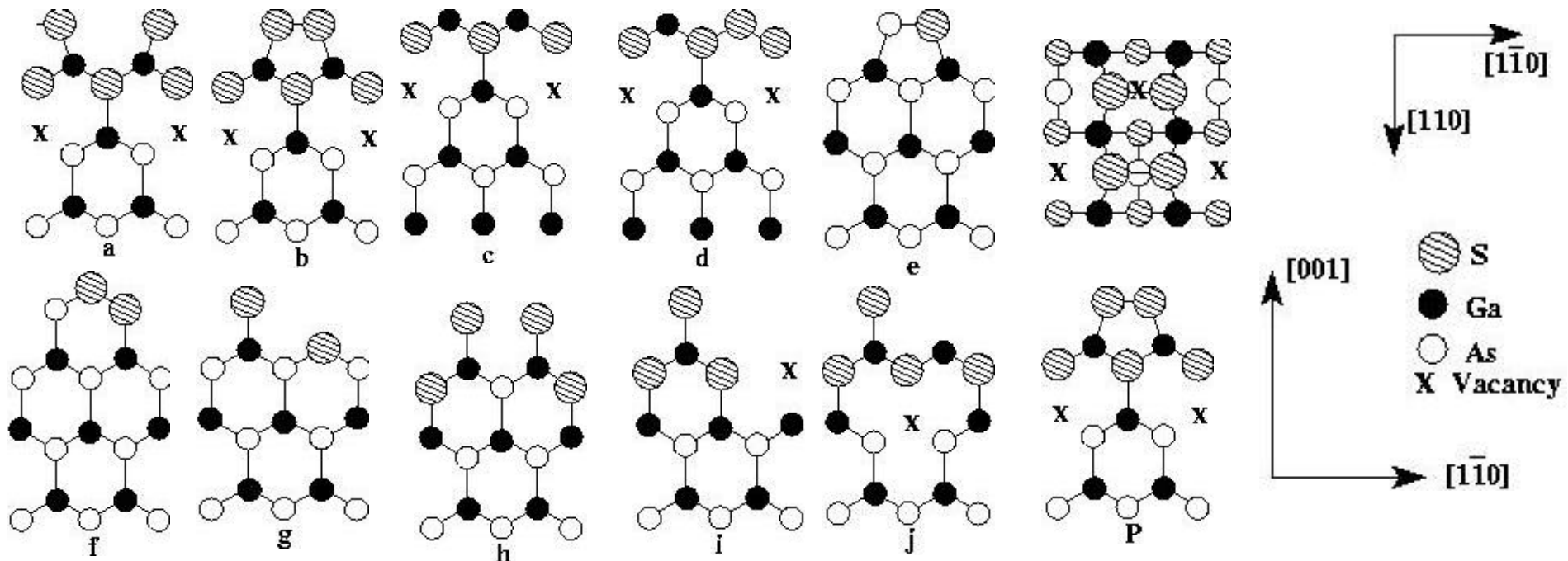




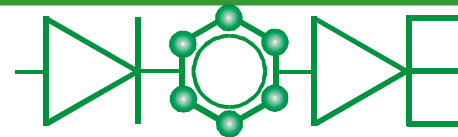
S:GaAs(100)



- PTCDA films on S:GaAs(100) show the best structural properties.[1]
- LEED and RHEED suggest (2x1) reconstruction.[2]
- Based on XPS and RAS: S-S, Ga-S dimer pairs as well as S-As surface bonding depending on initial surface.
- Se:GaAs(100) and S:GaAs(100) should be similar .

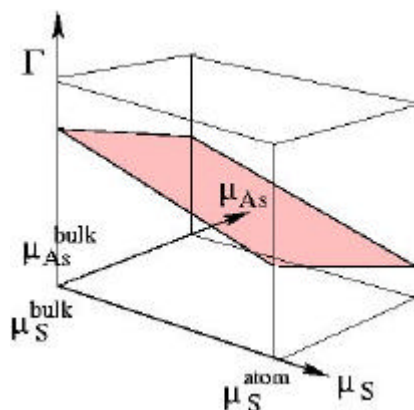
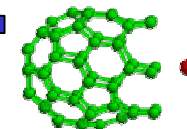


[1] Kampen et al. Appl.Surf.Sci. **175-176**, 326 (2001) [2] Park et al. Appl. Phys. Lett. **79**, 4124 (2001)





S:GaAs(100)

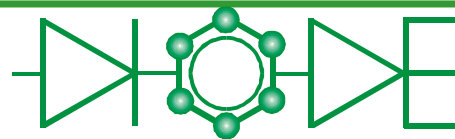
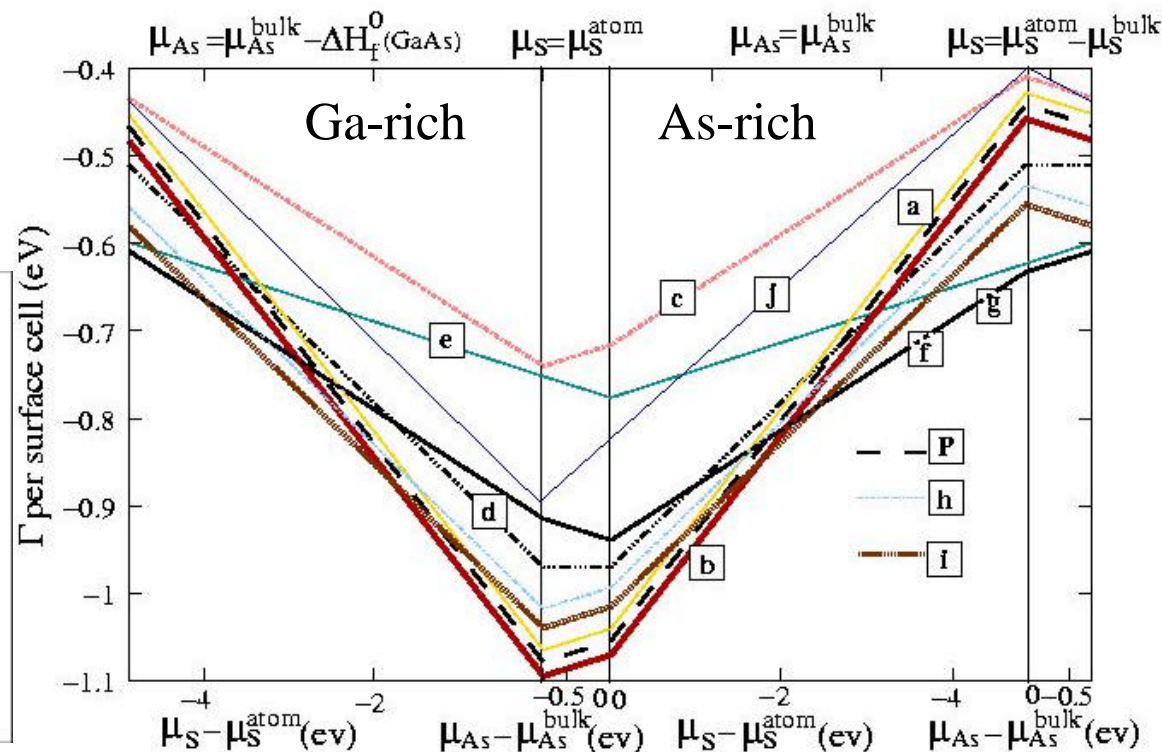
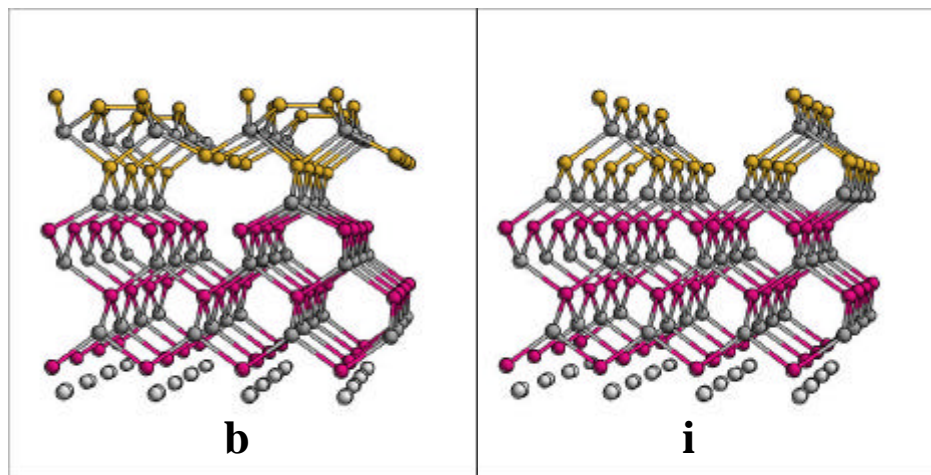


Several structures compared by surface energy calculation, (depending on the S and As chemical potential).

$$G = E_{\text{tot}} - \sum m_i N_i$$

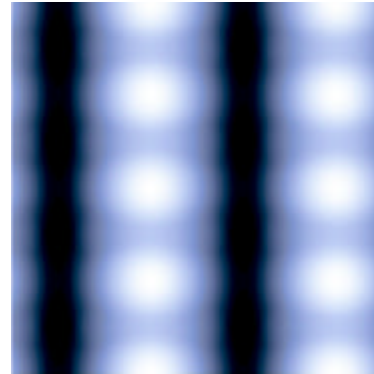
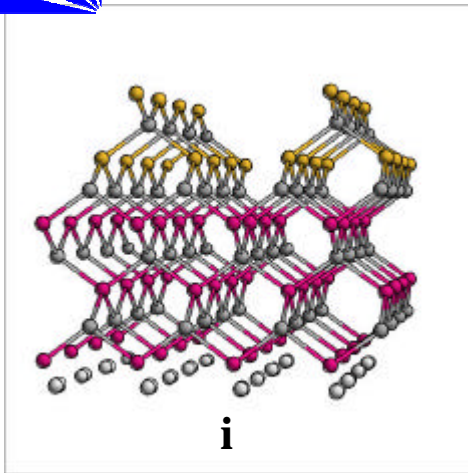
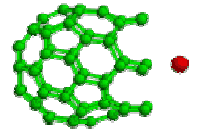
$$m_{\text{Ga}} + m_{\text{As}} = m_{\text{GaAs}}^{\text{bulk}} \quad m_{\text{GaAs}}^{\text{bulk}} = m_{\text{Ga}}^{\text{bulk}} + m_{\text{As}}^{\text{bulk}} - \Delta H_f^0(\text{GaAs})$$

$$G = E_{\text{tot}} - m_{\text{GaAs}}^{\text{bulk}} N_{\text{Ga}} - m_{\text{As}}^{\text{bulk}} (N_{\text{As}} - N_{\text{Ga}}) - m_{\text{S}}^{\text{atom}} N_{\text{S}} - (m_{\text{As}} - m_{\text{Ga}}) (N_{\text{As}} - N_{\text{Ga}}) - (m_{\text{S}}^{\text{bulk}} - m_{\text{S}}^{\text{atom}}) N_{\text{S}}$$

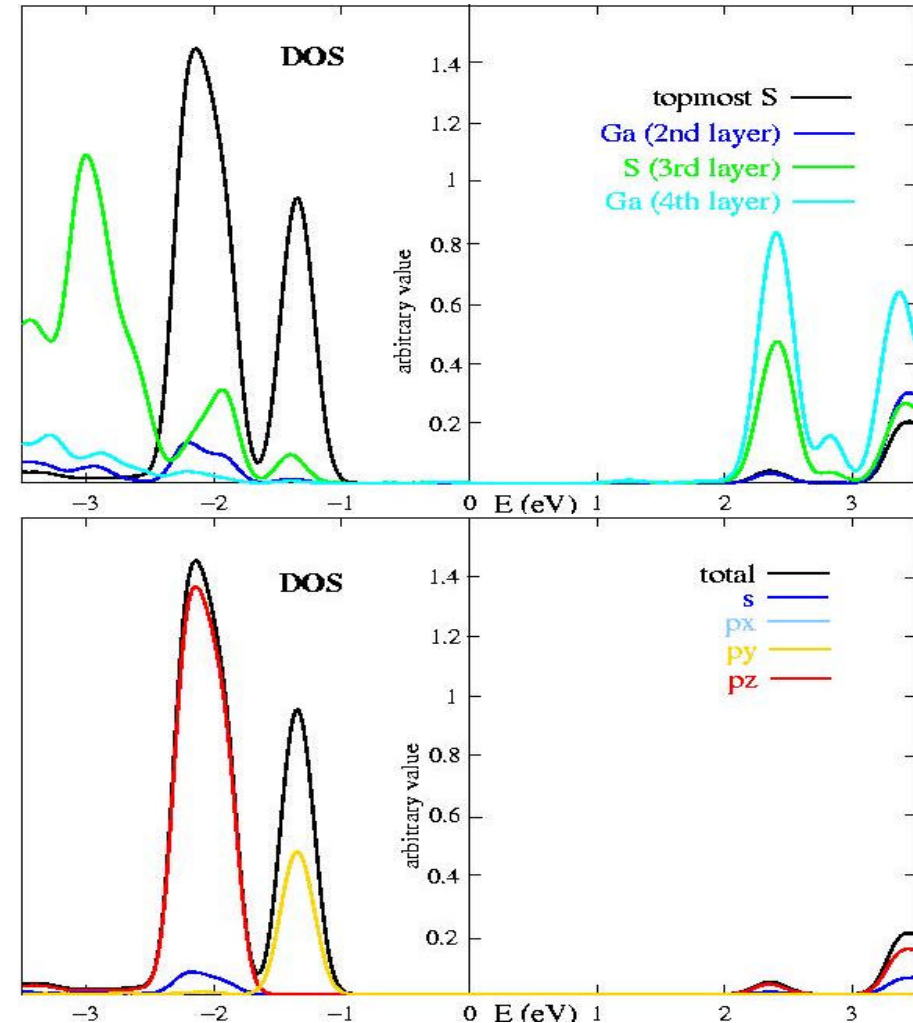




S:GaAs(100)



- For the Ga rich case: structures with gallium – sulphide like overlayer (*b,i*) found to be most stable.
- XPS suggest top and sublayer sulphur atoms [3]
- Compared with the XPS results (two layers of S with similar bonding type) *i* structure is more likely to exist .
- *i* shows good semiconducting properties.
- Se:GaAs(100) and S:GaAs(100) are similar.[4]
- Both surfaces well passivated.

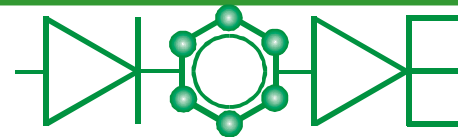


[3] Zahn et al. Vacuum **57** , 139-144 (2000)

[4] Gonzalez et al. Madrid



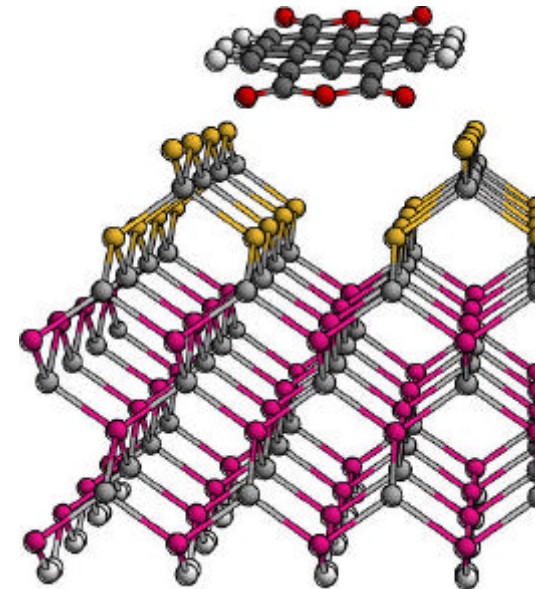
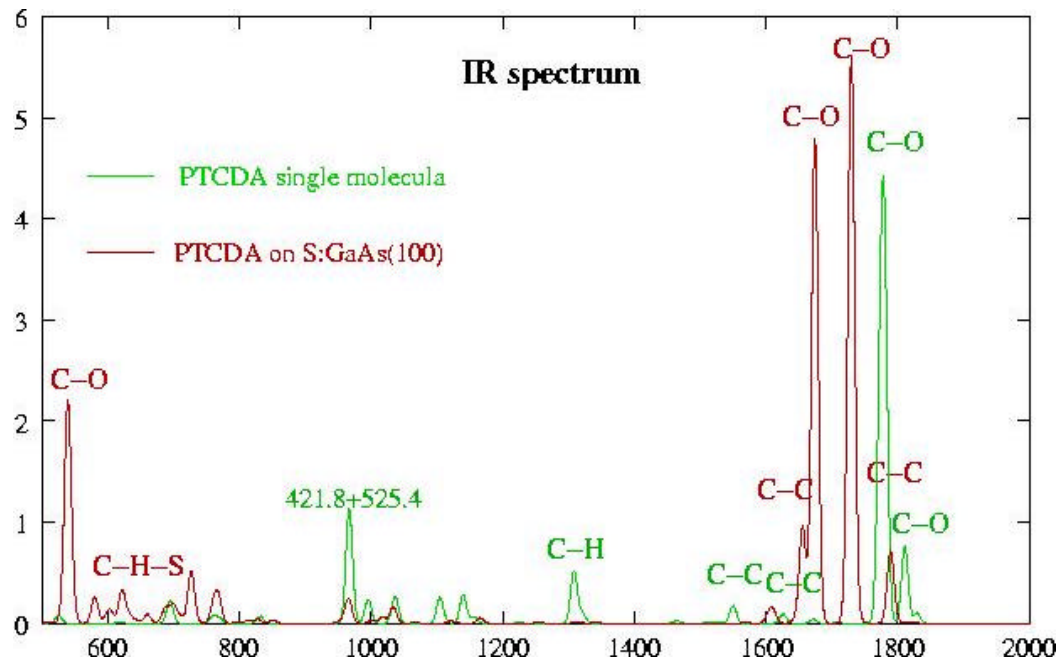
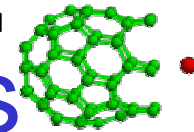
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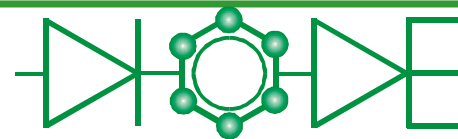
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Single PTCDA molecule on S:GaAs

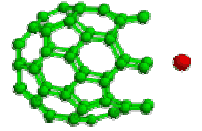


- The most stable position of one PTCDA molecule on the *i* reconstructed S:GaAs.
- The PTCDA molecule enclose an $\sim 10^\circ$ angle with surface, parallel to the top S rows.
- In the IR spectrum of the adsorbed molecule the C-O peak shifted, and increased.
- Interaction between the surface S and the O of the PTCDA.
- In the adsorbtion of the PTCDA Van der Waals interaction plays an important role.





Conclusion



- The structure of S passivated GaAs(100) surface has been identified. For the Ga rich case we found structures with gallium-sulfide like overlayer. Compared with the experimental results we suggest a (2x1) reconstruction, with single S atoms in the top layer and with third S-sublayer.
- The Se:GaAs(100) and S:GaAs(100) surface show similarities.
- Both structure give rise to a semiconducting surface.
- In the adsorption of the PTCDA molecule to the S:GaAs surface Van der Waals interaction plays an important role.
- In the IR spectrum of the adsorbed molecule the C-O peak increases and shifts, because of the interaction between the surface S and O of the PTCDA.

Outlook : •PTCDA layers on the S:GaAs(100).

- To describe the transport properties Green function approach.
- DFTB can be efficiently coupled to Green function techniques (Aldo di Carlo). [5]

[5] Frauenheim et al. J.Phys.:Condens. Matter. **14** (2002) 3015-3047

