(Applied) Theory:
core level spectroscopy of surface species

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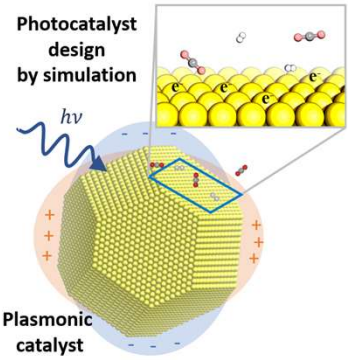
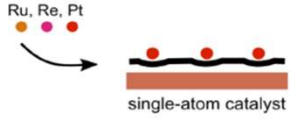
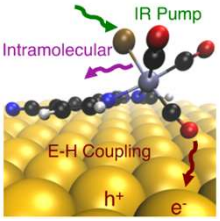
Computational Surface Science group

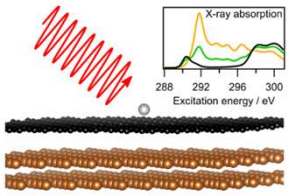


Design of functional nanostructures



Ultrafast energy transfer & surface spectroscopy





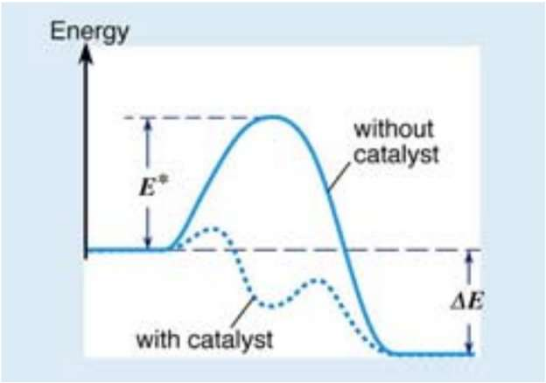
Surface Science

Nobel Prize for Gerhard Ertl

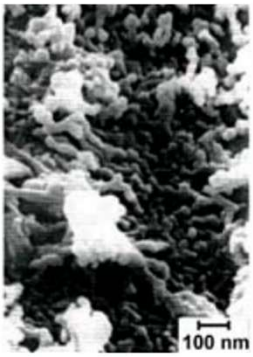
The Nobel Prize in Chemistry 2007 was awarded to Gerhard Ertl "for his studies of chemical processes on solid surfaces"

Catalysis …it's complicated

A good principle



The ugly reality



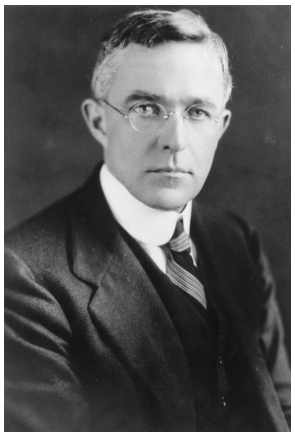
Technical conditions: T ~ 400°C, p ~ 300 bar
promoted iron catalyst

BASF S6-10 catalyst (at. %)

	Fe	K	Al	Ca	O
Bulk composition	40.5	0.35	2.0	1.7	53.2
Surface –					
unreduced	8.6	36.2	10.7	4.7	40.0
reduced	11.0	27.0	17.0	4.0	41.0
cat. active spot	30.1	29.0	6.7	1.0	33.2

Mittasch catalyst to generate ammonia via the Haber-Bosch process

Irving Langmuir's idea, Nobel Prize 1932



"Most finely divided catalysts must have structures of great complexity. In order to simplify our theoretical consideration of reactions at surfaces, let us confine our attention to reactions on plane surfaces. If the principles in this case are well understood, it should then be possible to extend the theory to the case of porous bodies. In general, we should look upon the surface as consisting of a checkerboard …"

The "surface science approach" is enabled by

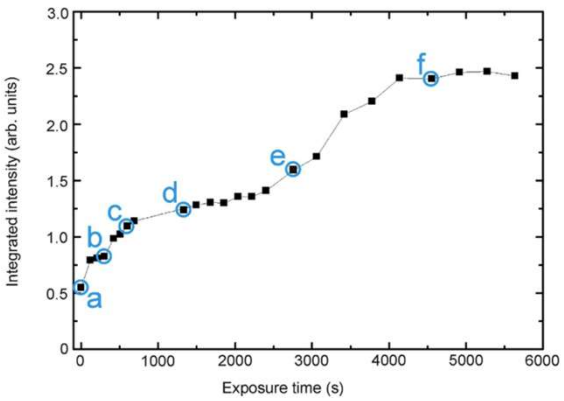
UHV

clean **sample preparation**

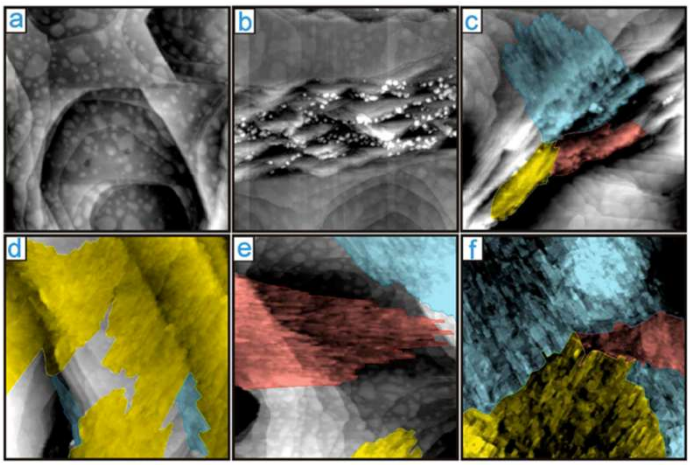
and **surface-sensitive methods**

Surface Science in Action: Oxidation of Ruthenium

integral intensity of O 1s in XPS



Oxygen uptake on Ru(0001),
dosing 3 × 10^{-5} mbar of O_2 at 680 K

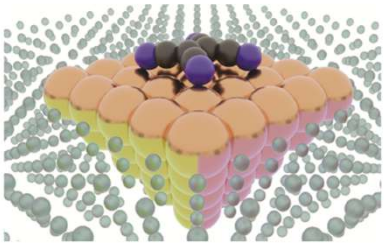


Herd, Knapp, Over, J. Phys. Chem. C 2012, 116, 24649–24660

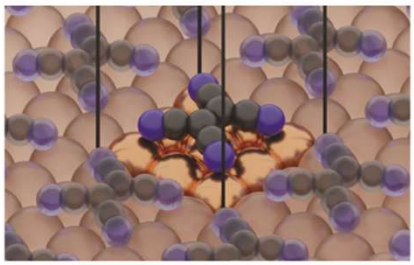
Computational Surface Science

Modelling surfaces and interfaces with electronic structure theory methods

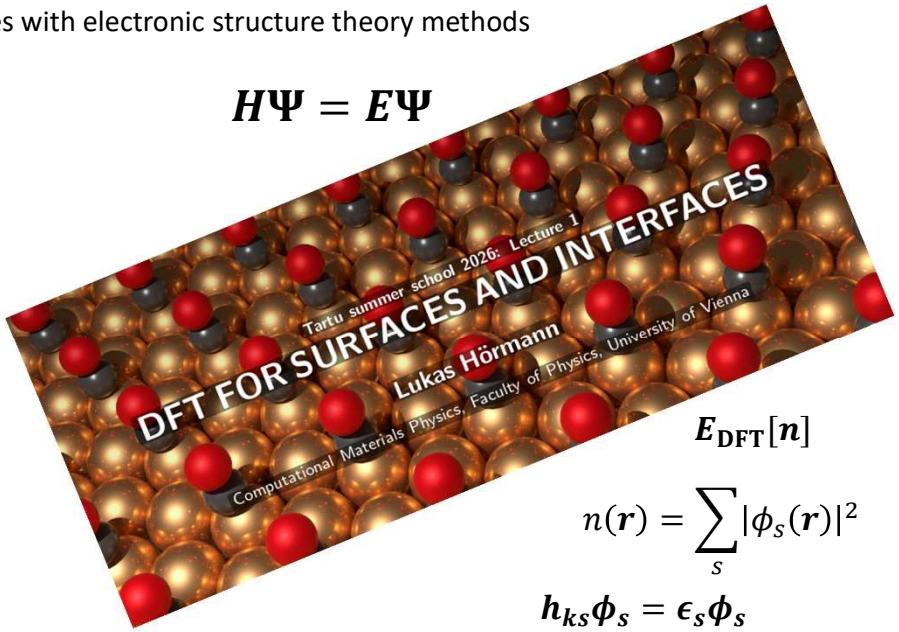
Cluster model



Repeated slab model



$$H\Psi = E\Psi$$



$$E_{\mathrm{DFT}}[n]$$

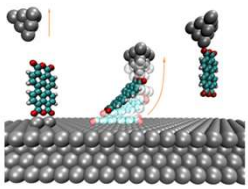
$$n(r) = \sum_s |\phi_s(r)|^2$$

$$h_{ks}\phi_s = \epsilon_s\phi_s$$

Computational Surface Science Applications

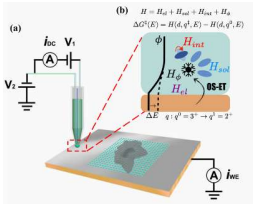
Surface Nanoassembly

Surface Nanofabrication



Science Advances (2021)

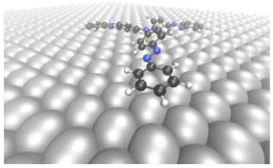
Nanoelectrochemistry



Nature Commun. (2021)

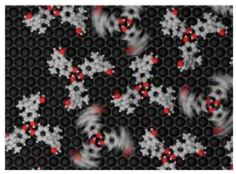
Functional Interfaces

Molecular Switches



PRL 116, 027201 (2016)
JPCL 7, 2080-2084 (2016)
J. Phys: CM 31, 044003 (2018)

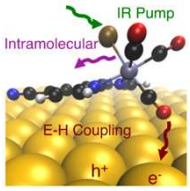
Molecular Rotors



Nano Lett. 16, 1884–1889 (2016)

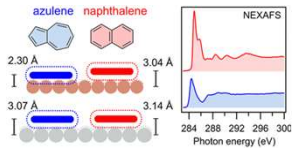
Surface Spectroscopy

Ultrafast energy transfer



PRB 94, 115432 (2016)
JPCL 9, 406-412 (2018)

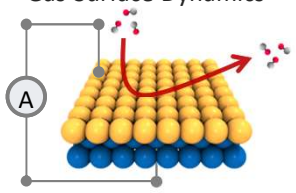
Spectroscopic Signatures



PRX 9, 011030 (2019)
Chem. Matter 32, 1041-1053 (2020)
Angew. Chem. Int Ed (2025)

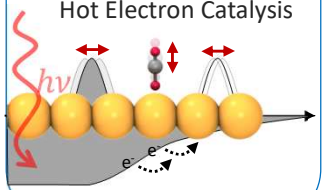
Catalysis

Nonadiabatic Effects in Gas-Surface Dynamics



PRL 118, 256001 (2017)
Chem. Sci. 10, 1089-1097 (2019)

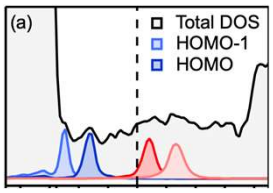
Hot Electron Catalysis



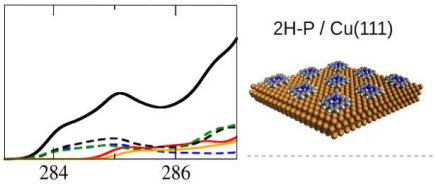
JACS Au (2021), Nanoscale (2021)

Simulating Structure, Stability, Chemical Bonding at Surfaces

Electronic Structure

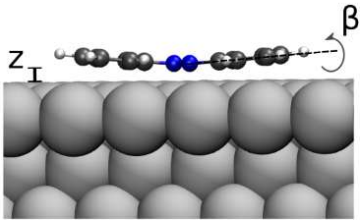


Charge transfer, energy level alignment hybridisation



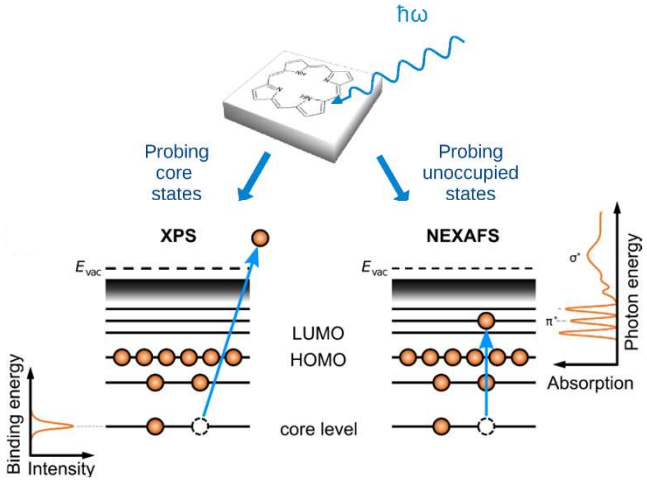
XPS/NEXAFS

Adsorption Structure



We have to get the surface structure, the electronic structure, and the spectroscopy right

Measuring signatures of surface chemistry



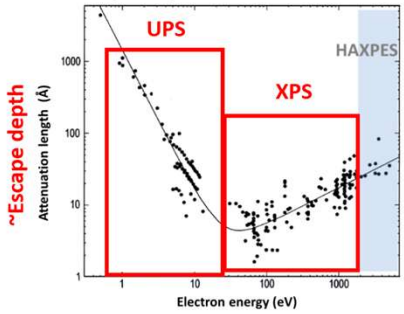
Klein et al., J. Phys.: Condens. Matter 33, 154005 (2021)

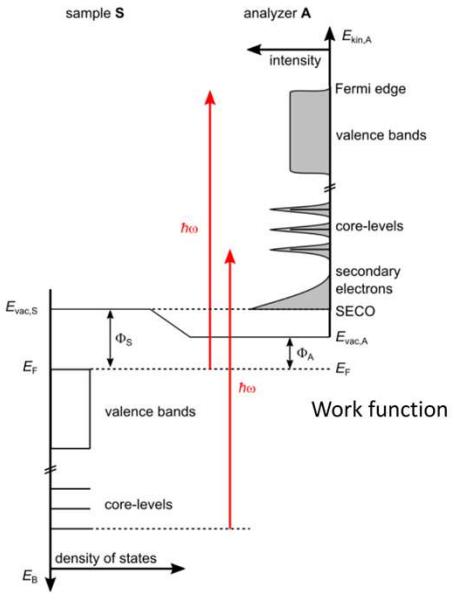
Diller et al., J. Chem. Phys. 146, 214701 (2017)

Photoelectron Spectroscopy: The ultimate surface science tool

$$E_{\mathrm{kin}} = \hbar\omega - \Phi - E_{\mathrm{B}}$$

- Photoemission of electrons from the material
- Analysis of the kinetic energy distribution of the electrons
- Either in the gas phase (rare) or on surfaces (mostly)
- There is always a surface involved, because the electrons have to leave the material
- **And their escape depth is small**





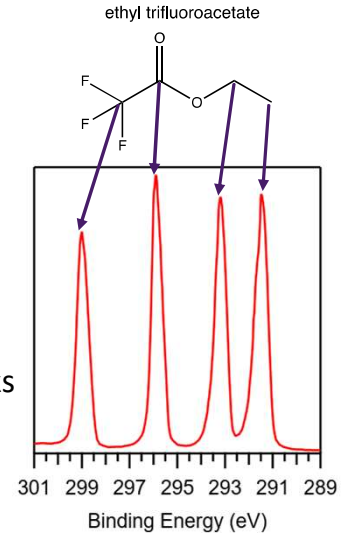
11

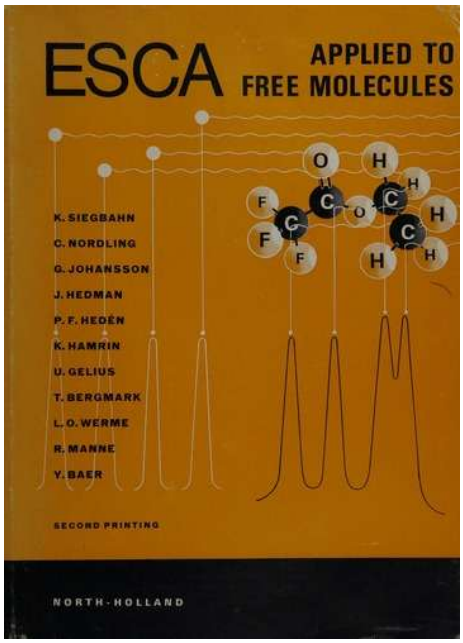
Problem 1: Relative Peak assignment

ETFA

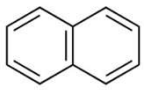
C1s XPS

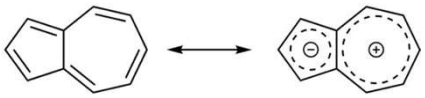
- Multiple chemical environments
- Clearly resolved peaks





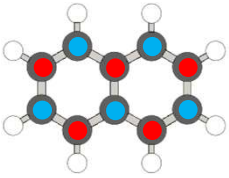
Topology and Spectroscopy





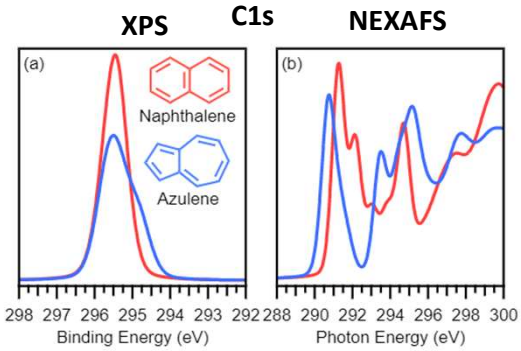
Naphthalene (Np)

Azulene (Az)



alternant

non-alternant



Klein et al., Phys. Rev. X 9, 011030 (2019)

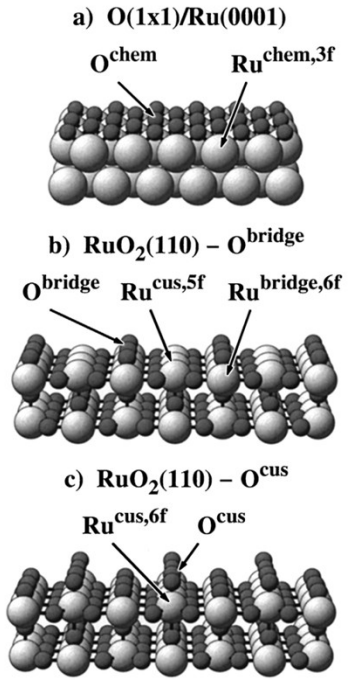
O/Ru(0001) vs. RuO_2

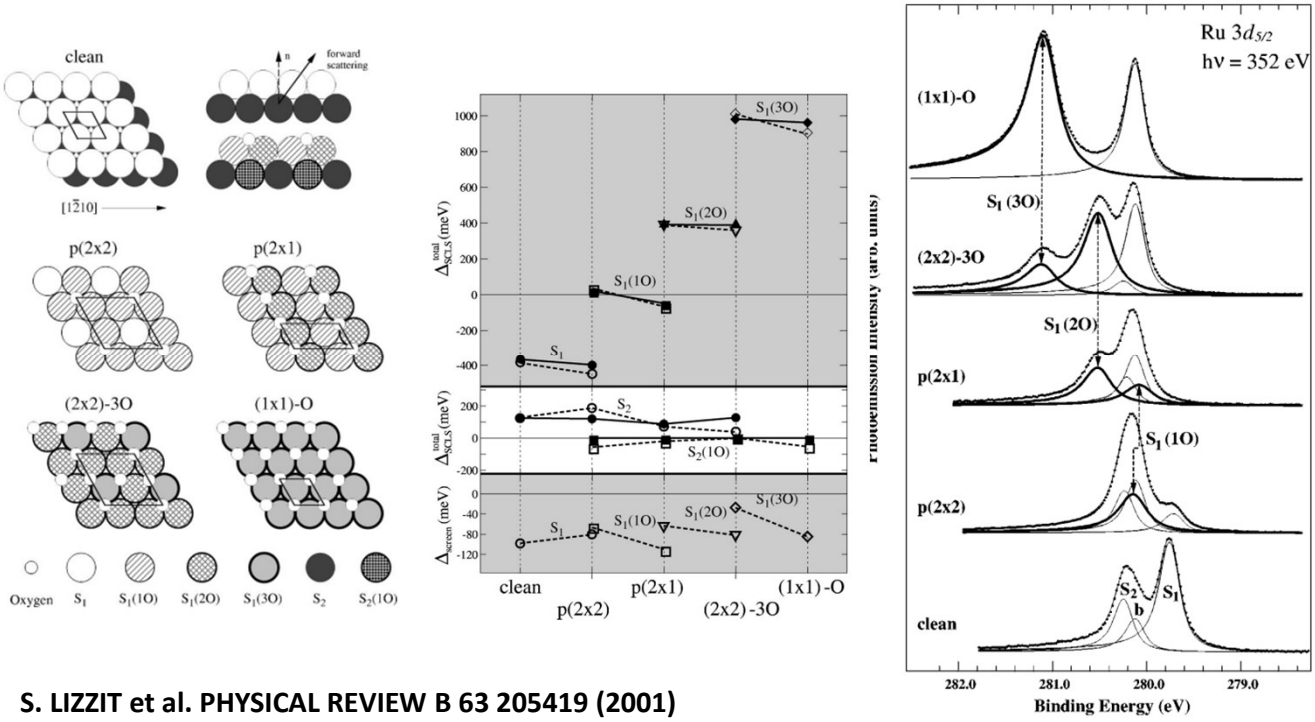
Table 1
Calculated Ru 3d and O 1s SCLSs on RuO_2(1 1 0)

Termination		Total	Screening	Initial
Ru 3d SCLSs in eV				
O^{bridge}	$Ru^{bridge,6f}$	+0.29	−0.15	+0.44
	$Ru^{cus,5f}$	−0.16	−0.02	−0.14
O^{cus}	$Ru^{bridge,6f}$	+0.40	−0.14	+0.54
	$Ru^{cus,6f}$	+1.37	+0.07	+1.30
O 1s SCLSs in eV				
O^{bridge}	O^{bridge}	−0.87	−0.68	−0.19
O^{cus}	O^{bridge}	−0.97	−0.77	−0.20
	O^{cus}	−0.79	−0.98	+0.19

Shown are the total shifts, as well as their decomposition into screening and initial state parts: $\Delta^{total}_{SCLS} = \Delta^{screen} + \Delta^{initial}_{SCLS}$.

Reuter, Scheffler, Surf. Sci. 490 (2001), 20-28





S. LIZZIT et al. PHYSICAL REVIEW B 63 205419 (2001)

DeltaSCF for XPS

The SCLS, Δ_{SCLS}, is defined as the difference in energy that is needed to remove a core electron either from a surface or from a bulk atom,

$$\Delta_{SCLS}=[E^{surface}(n_c-1)-E^{surface}(n_c)] -[E^{bulk}(n_c-1)-E^{bulk}(n_c)], \quad (1)$$

where $E^{surface(bulk)}(n_c)$ is the total energy of the system considered as a function of the number of electrons n_c in a particular core level c of a surface or bulk atom, respectively.[9] Within the initial state approximation, $\Delta^{initial}_{SCLS}$ is given by

$$\Delta^{initial}_{SCLS}\approx-[\epsilon_c^{surface}(n_c)-\epsilon_c^{bulk}(n_c)]. \quad (2)$$

Here, $\epsilon_c^{surface}$ and ϵ_c^{bulk} are the Kohn-Sham eigenvalues of the particular core state c, so that in this approximation the SCLS is simply due to the variation of the orbital eigenenergies before the excitation of the core electron. A full calculation of the ionization energy, which includes the screening contributions from the valence electrons in response to the created core hole, can be achieved by calculating the total energy of an impurity with a core hole in the selected core state. The SCLS is then the difference of two total energies, with the impurity located once at the surface and once inside the bulk.[27] To a good approximation, this difference can also be obtained via the Slater-Janak transition state approach of evaluating total energy differences.[28] Using the mean value theorem of integration,

$$E(n_c-1)-E(n_c)=\int_{n_c}^{n_c-1}\frac{\partial E(n')}{\partial n'}dn'\approx-\epsilon_c(n_c-1/2), \quad (3)$$

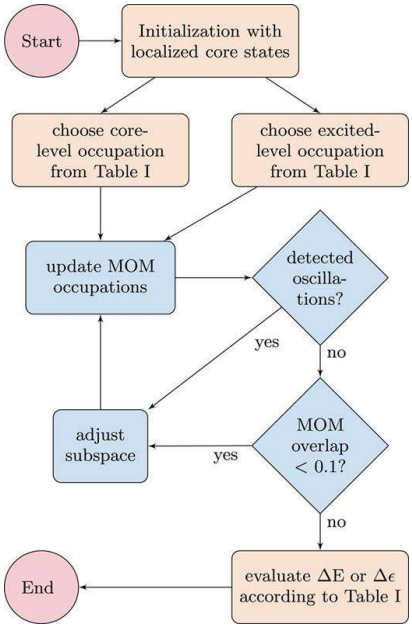
Equation (1) can be cast into the form of Eq. (2), but this time with a core-level occupation of $n_c-1/2$. Note that this latter approach, from which we derive what we will henceforth call the total SCLS, takes both initial and final state effects (in the spectroscopic sense) into account, so that the results can be compared with the experimental values.

S. LIZZIT et al. PHYSICAL REVIEW B 63 205419

DeltaSCF for XAS

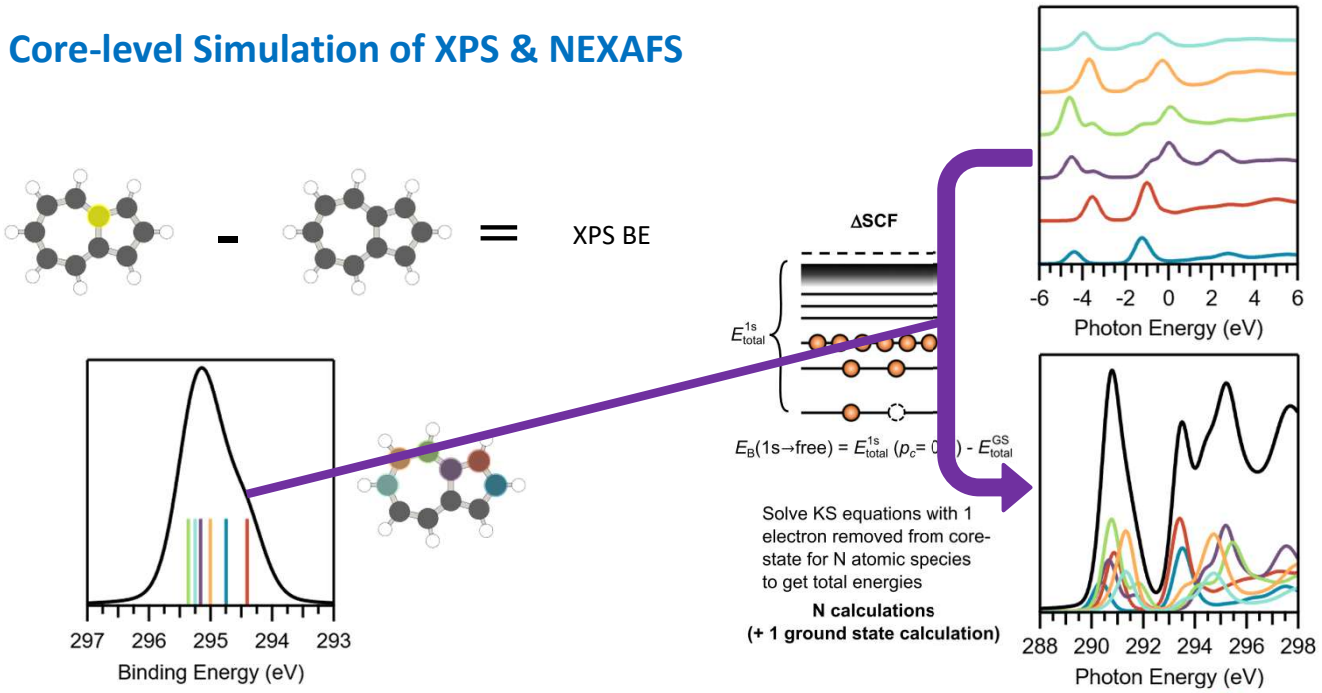
$$\Delta E_{\Delta\mathrm{SCF}} = E_\mathrm{f} - E_\mathrm{i} = E\left(q_\mathrm{c} = 0, q_\mathrm{v} = 1\right) - E\left(q_\mathrm{c} = 1, q_\mathrm{v} = 0\right)$$

		explicit			implicit			neutral implicit		
		GS	ΔSCF‡	TS‡	GTS‡	FCH	TP	GTP	XCH	XTP	XGTP
		$\Delta\epsilon$	ΔE	$\Delta\epsilon$	$\Delta\epsilon$	$\Delta\epsilon$	$\Delta\epsilon$	$\Delta\epsilon$	$\Delta\epsilon$	$\Delta\epsilon$	$\Delta\epsilon$
core	q_c	1	0	½	⅓	0	½	⅓	0	½	⅓
virtual	q_v	0	1	½	⅔	0	0	0	1	½	⅔



J. Chem. Phys. 150, 074104 (2019)

Core-level Simulation of XPS & NEXAFS



T. Mizoguchi, I. Tanaka, S. Gao and C. J. Pickard, *J. Phys. Condens. Matter* **21**, 104204 (2009)
B. P. Klein, S. J. Hall and R. J. Maurer, *J. Phys. Condens. Matter* **33**, 154005 (2021)

CASTEP

FHI-aims
The ab initio materials simulation package

Codes

CASTEP

CASTEP XPS and NEXAFS Tutorial

This tutorial explains how to calculate and decompose XPS and NEXAFS spectra for molecule-metal adsorbed systems using the DFT software CASTEP.

All tools needed to generate XPS and NEXAFS spectra can be found in the CASTEP section of the core-level-spec-tools repository on the Maurer Group Github (https://github.com/maurergroup/core-level-spec-tools). Included in this are several tools to help in this process:

- *autoscript.py* - Python script which will generate all XPS and NEXAFS input files
- *core_excitation.py* - Code in which the autoscript will use
- *castep_get_XPS_energies.py* - Python script to calculate the XPS binding energies
- *plot_xps.py* - Python script to sum up XPS peaks and broaden into a spectrum
- *execute_molpdos.sh* - Bash script to run MolPDOS for all angles and atoms
- *plot_nexafs.py* - Python script to process MolPDOS output data into a broadened NEXAFS spectra
- *plot_mo.py* - Python script to process MolPDOS output data into MO orbital spectra

www.fhi-aims.org

FHI-aims tutorials

FHI-aims
The ab initio materials simulation package

Back to top

Electronic Excited States

RPA, GW, and BSE for Molecules and Solids

This tutorial focuses on many-body perturbation theory methods "beyond DFT" in FHI-aims. In particular, three main approaches are discussed:

a. The GW approximation for quasiparticle properties (i.e., charged excitations such as "electrons" and "holes" in semiconductors);

b. The random-phase approximation (RPA) to electron correlation energies, for total energies;

c. The Bethe-Salpeter equation (BSE) based on GW, for neutral (e.g., optical) excitation energies (in FHI-aims, currently available for non-periodic simulations of molecules).

MP2 and Coupled Cluster for Solids (and Molecules) - the Interface `CC-aims` to `CC4S`

The interface `CC-aims` in FHI-aims allows to use the coupled cluster code CC4S. The tutorial demonstrates the needed steps to get from a FHI-aims calculation to start a calculation with CC4S. CC4S enables the calculation of:

- MP2
- CCSD

Real-Time TDDFT and Ehrenfest Dynamics

A tutorial providing an overview on running RT-TDDFT simulations for both isolated and periodic systems within FHI-aims, including a basic review of the theory and all inputs needed to run the simulations. The tutorial also covers running RT-TDDFT with Ehrenfest dynamics and necessary inputs.

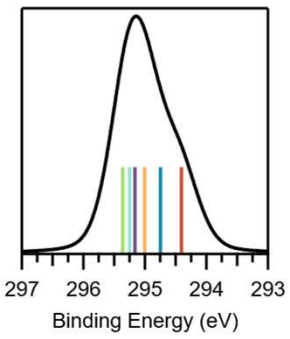
Core Level Spectroscopy with ΔSCF

A comprehensive tutorial on how to perform ΔSCF calculations for simulation of x-ray spectroscopy within FHI-aims using force_occupation_basis and force_occupation_projector for periodic and aperiodic systems.

https://github.com/maurergroup/deltascf-aims

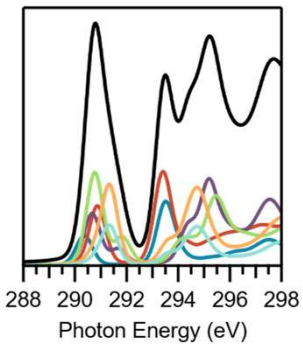
Unpicking spectral contributions

XPS

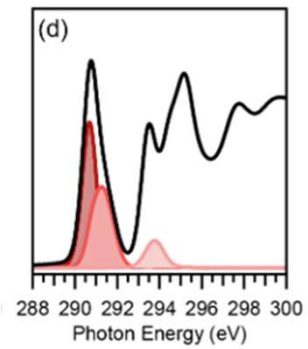


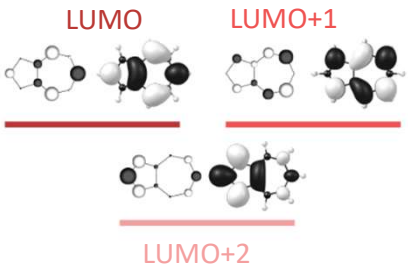
NEXAFS

Initial states



Final states





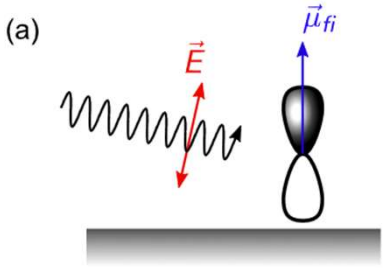
Hall et al., J. Phys. Chem. C 127, 1870–1880 (2023)

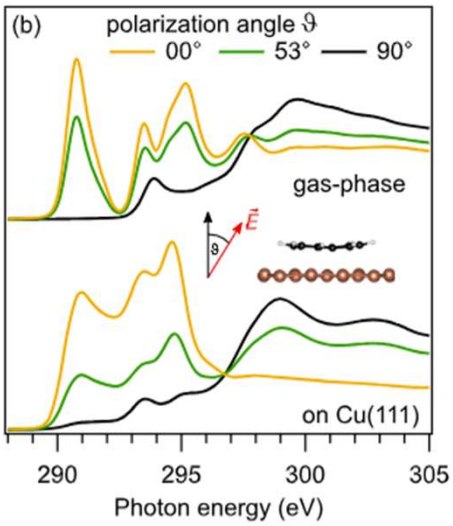
Klein et al., J. Phys. Condens. Matter 33, 154005 (2021)

Orientational/polarization dependence

$$\sigma_i(h\nu) \propto \sum_f |\langle\psi_f|\mathbf{e}\cdot\mathbf{p}|\psi_i\rangle|^2 \delta(h\nu - \underbrace{(E_f - E_i)}_{\Delta E_{fi}})$$

$$\mu_{fi} = |\langle\psi_f|\mathbf{e}\cdot\mathbf{p}|\psi_i\rangle|^2 \approx |\mathbf{e}\cdot\underbrace{\langle\psi_f|\mathbf{p}|\psi_i\rangle}_{\mathbf{D}_{fi}}|^2$$



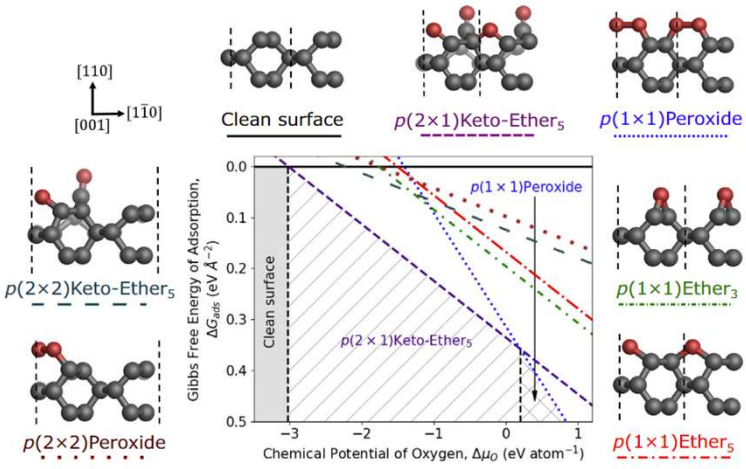


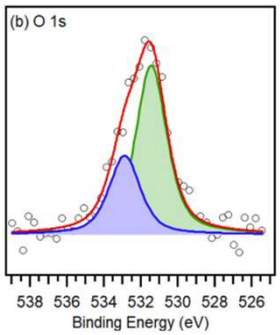
Klein et al., J. Phys. Condens. Matter 33, 154005 (2021)

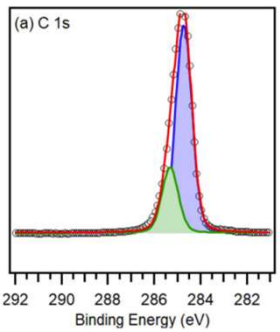
Problem 2: Absolute referencing of binding energies

FHI-aims
The ab initio materials simulation package

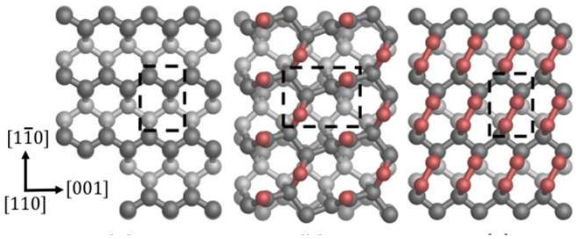
Example: Oxygen surface terminations of polished and acid-etched diamond (110)

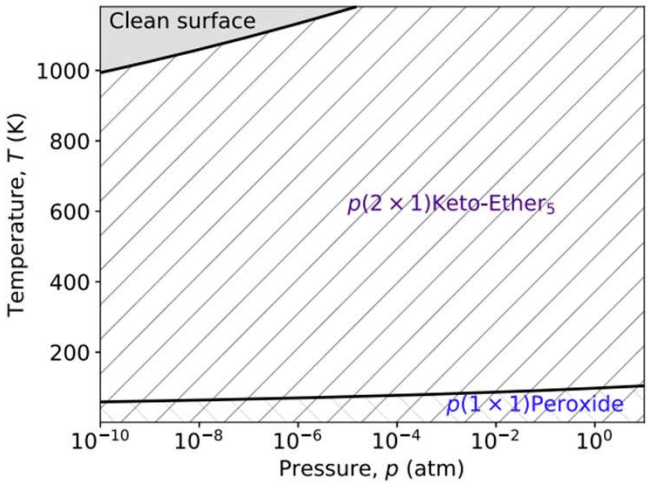






Chaudhuri, Hall, et al., Communications Materials **3**, 6 (2022)





C 1s ΔBE (eV)

	Simulation		Experiment		
Species	***p*(2 × 1)**	***p*(2 × 2)**	**This Work**	**Baldwin[48]**	**Makau[47]**
C=O	1.16	0.74	0.7	4.5	2.2
C-O-C	1.46	0.80	0.7	1.9	1.1
C-O-C	1.23	0.30	0.7	1.9	1.1

O 1s ΔBE (eV)

Simulation		Experiment		
***p*(2 × 1)**	***p*(2 × 2)**	**This Work**	**Baldwin[48]**	**Makau[47]**
1.00	1.31	1.5	2.1	1.7

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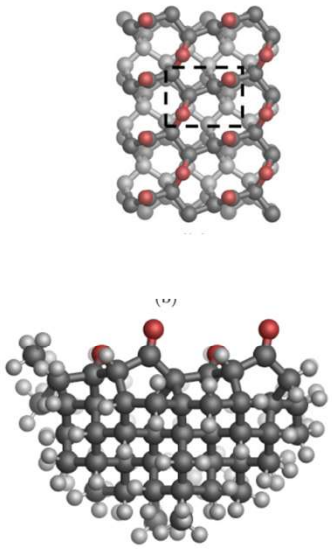
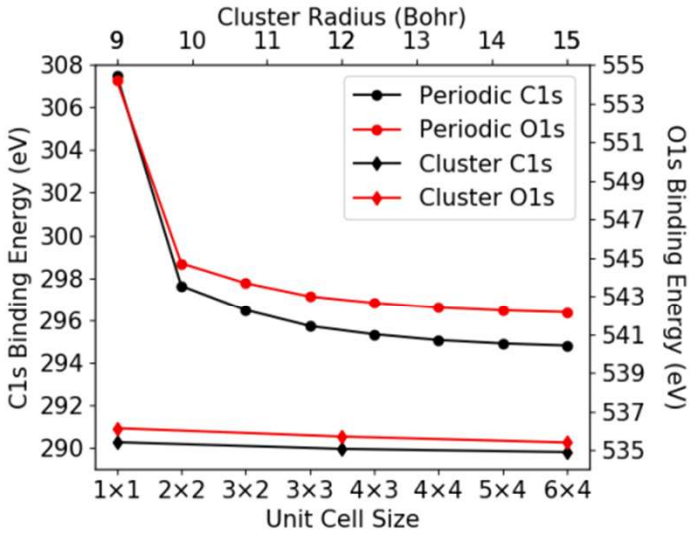
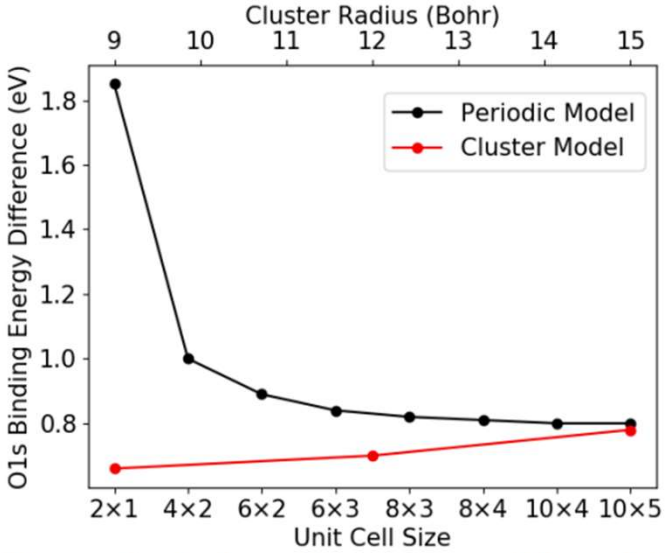




Supplementary Figure 7. Graph showing the convergence of simulated absolute carbon 1 (C 1s) and oxygen 1s (O 1s) binding energies of the $p(1 \times 1)$Peroxide phase using periodi and cluster models, calculated via CASTEP and FHI-aims respectively.

24



Supplementary Figure 8. Graph showing the convergence of the simulated O 1*s* binding energy difference between the carbonyl and ether groups in the $p(2 \times 1)$Keto–Ether$_5$ phase using periodic and cluster models, calculated via CASTEP and FHI-aims respectively.

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Core Electron Binding Energies in Solids from Periodic All-Electron Δ-Self-Consistent-Field Calculations

J. Matthias Kahk, Georg S. Michelitsch, Reinhard J. Maurer, Karsten Reuter, and Johannes Lischner*

Cite This: *J. Phys. Chem. Lett.* 2021, 12, 9353–9359

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FHI-aims
The ab initio materials simulation package

In principle, the binding energy of a core electron referenced to the energy of the highest occupied state could be obtained from the difference of the results of two ΔSCF calculations: one for the removal of a core electron and one for the removal of a valence electron. Subtracting these two removal energies yields

$$E_B = (E_{N,gs} - E_{N-1,ch}) - (E_{N,gs} - E_{N-1,gs}) = E_{N-1,gs} - E_{N-1,ch}$$

Table 1. Comparison of Calculated and Experimental Core Electron Binding Energies in Solids

solid	core level	theor E_B (eV)	expt E_B (eV)	ref	error[a] (eV)
Li	Li 1s	54.88	54.85	53−56	0.03
Be	Be 1s	111.88	111.85	57	0.03
Na	Na 1s	1071.56	1071.75	56, 58, 59	−0.19
	Na 2p	30.65	30.51		0.14
Mg	Mg 1s	1303.25	1303.24	57, 60−64	0.01
	Mg 2p	49.69	49.79		−0.10
graphite	C 1s	284.44	284.41	65−69	0.03
BeO	Be 1s	110.79	110.00		0.79
	O 1s	528.86	527.70	68, 70	1.16
hex-BN	B 1s	188.42	188.35	68, 71	0.07
	N 1s	396.39	396.00		0.39
diamond	C 1s	284.43	284.04	72−75	0.39
β-SiC	Si 2p	99.24	99.20	76−78	0.04
	C 1s	281.48	281.55		−0.07
Si	Si 2p	99.17	99.03	79, 80	0.14

[a]Mean absolute error = 0.24 eV.

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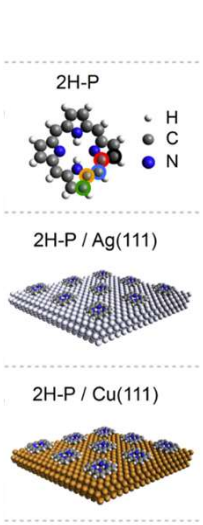
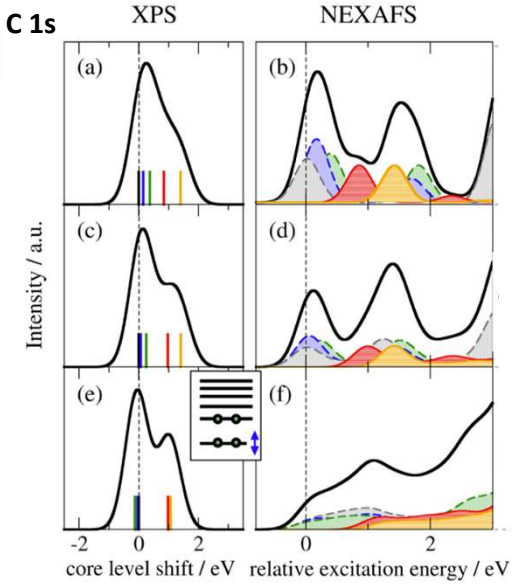
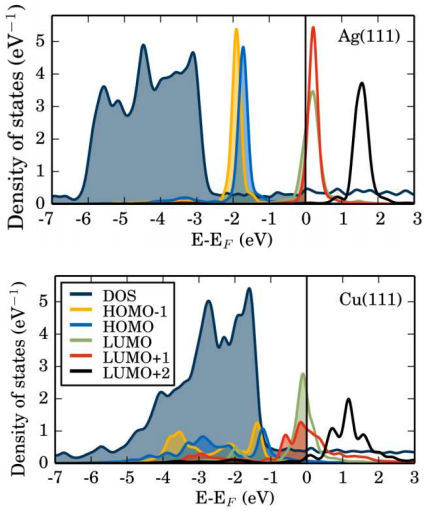
Surface Chemical Bonding – Quo Vadis?



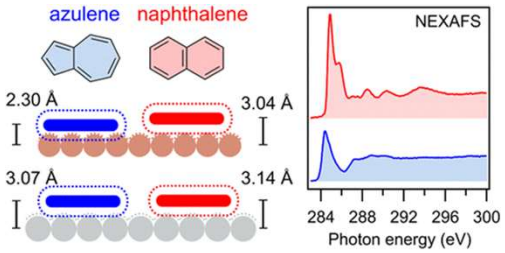




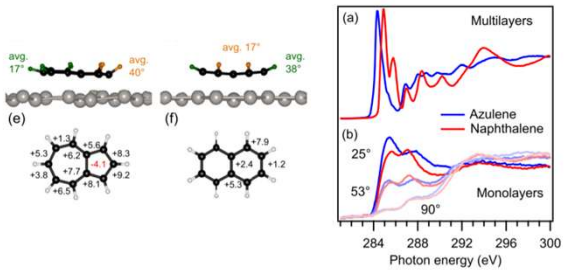
Hybridisation and charge transfer

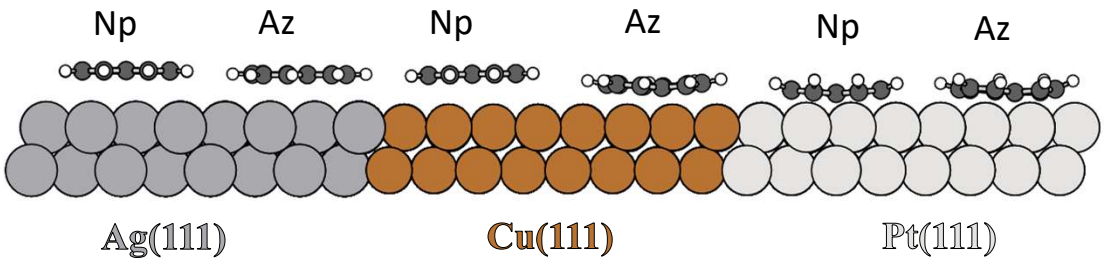
Müller, Diller, Maurer, Reuter, J. Chem. Phys. 144, 024701 (2016)
Diller et al., J. Chem. Phys. 146, 214701 (2017)

Naphthalene



Azulene





Detailed experiment/theory characterisation: XPS, NEXAFS, XSW, UPS, TPD, LEED, STM, AFM, DFT, ...

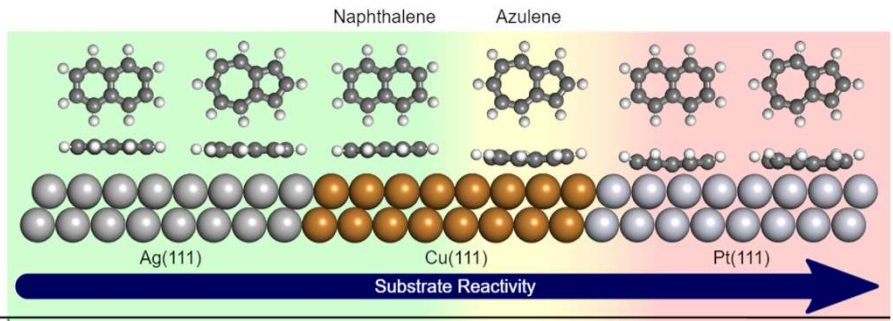
JPCC 123, 29219-29230 (2019) PRX 9, 011030 (2019) Chem. Matter 32, 1041-1053 (2020)


Michael Gottfried (Marburg)


Benedikt Klein


Sam Hall

Naphthalene & Azulene: a playground to understand surface chemistry

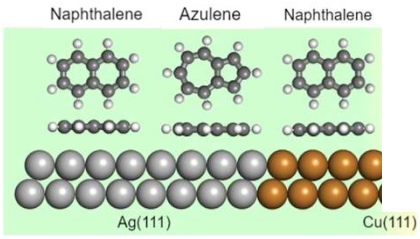


Adsorption Energy (kJ/mol)	118	128	135	173	298	335
Adsorption Height (Å)	3.10	2.94	2.96	2.33	2.09	2.10
Net Charge Transfer (e)	0.06	0.01	0.06	-0.49	0.03	0.02
Structural Deformation	None	None	None	Weak	Strong	Strong
Molecule-Metal Hybridisation	Weak	Weak	Weak	Intermediate	Strong	Strong

Category 1 **Category 2** **Category 3**

Hall et al., J. Phys. Chem. C 127, 1870–1880 (2023)

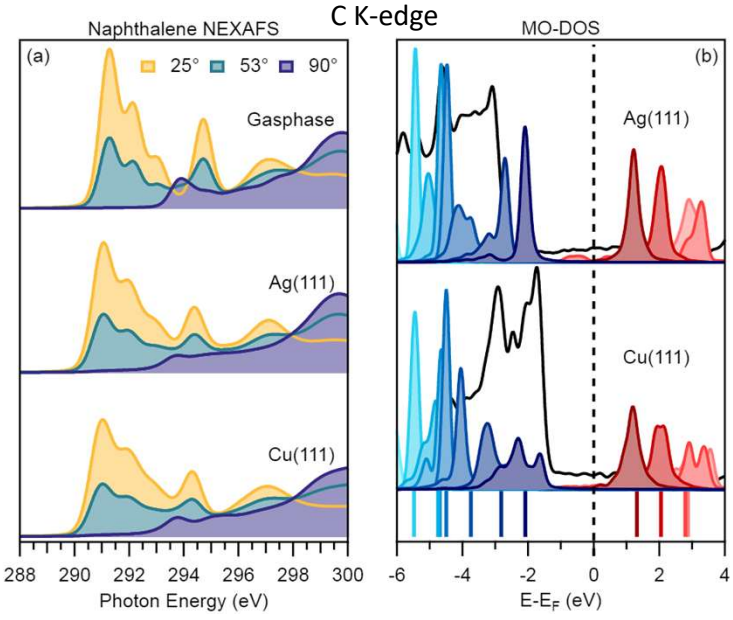
Category 1



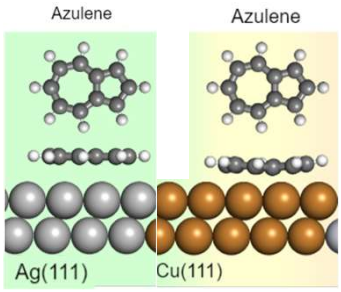
- No significant charge transfer
- Little hybridisation
- Spectra only slightly broadened
- Dichroism unaffected

"Physisorption"

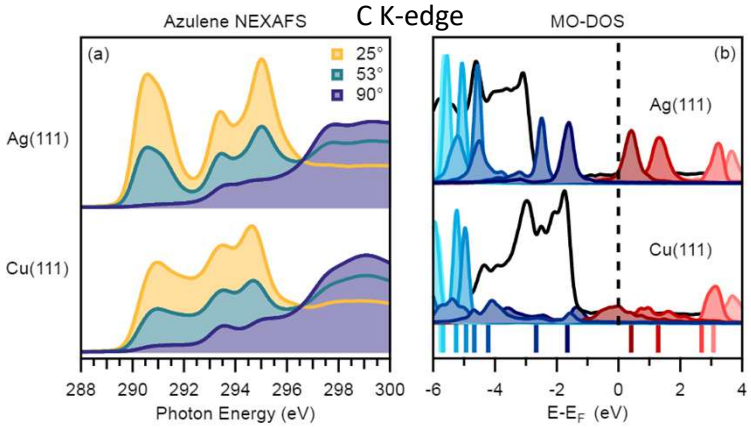
C K-edge



Category 2



C K-edge



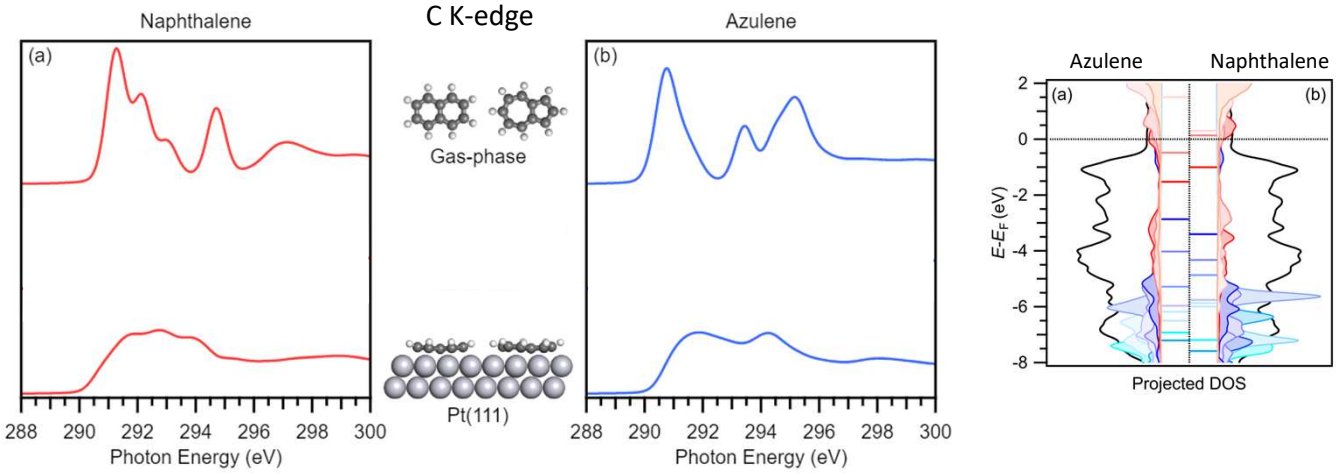
- Hybridisation for both Ag and Cu
- Only Az/Cu shows charge transfer
- Intensity of first peak diminished
- Dichroism also affected
- Neither clear case of “physisorption” nor “chemisorption”

Table 1: Relative intensities of the first 3 peaks seen in the NEXAFS spectra of azulene on Ag(111) and Cu(111) with respect to the corresponding peaks of azulene gas-phase spectrum.

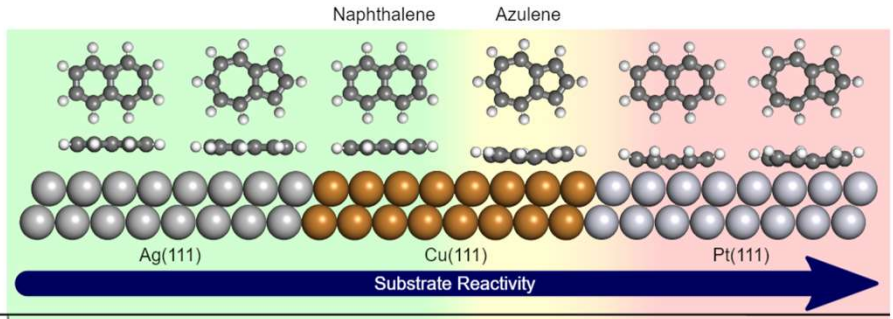
Peak	Relative Intensity	
	Az/Ag	Az/Cu
1	0.65	0.44
2	0.93	1.04
3	0.96	0.82

Charge Transfer

Category 3: “Chemisorption”



A playground to understand surface chemistry



Adsorption Energy (kJ/mol)	118	128	135	173	298	335
Adsorption Height (Å)	3.10	2.94	2.96	2.33	2.09	2.10
Net Charge Transfer (e)	0.06	0.01	0.06	-0.49	0.03	0.02
Structural Deformation	None	None	None	Weak	Strong	Strong
Molecule-Metal Hybridisation	Weak	Weak	Weak	Intermediate	Strong	Strong

Category 1 "Physisorption" **Category 2** Charge Transfer **Category 3** "Chemisorption"

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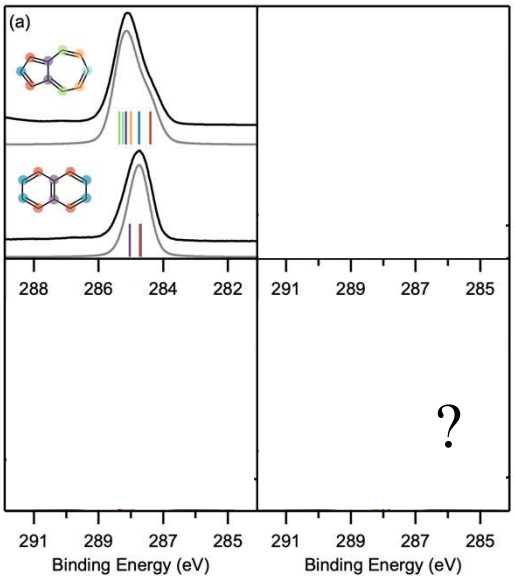
Accuracy of C1s XPS simulations



Prof. J Michael Gottfried

Dr. Benedikt Klein

Sam Hall

S. J. Hall, B. P. Klein and R. J. Maurer, arXiv:2112.00876

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The missing shoulder in Az on Ag(111)?

Sam Hall

- What is the cause of the loss of the shoulder in the XPS?

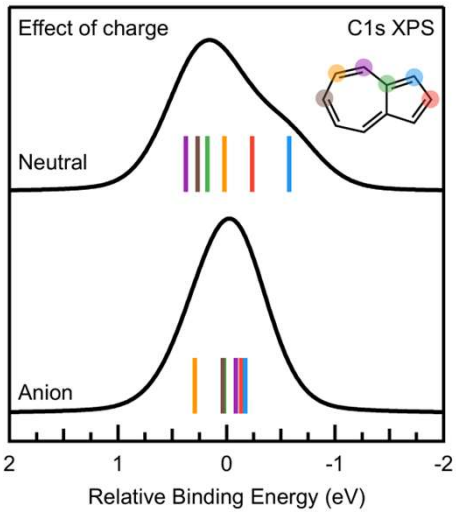
Method	Adsorption Height[1] / Å
Experiment (NIXSW)	2.98
DFT (PBE+D3)	2.94

  - Electrostatic artefact from finite size eff
  - Interaction with the metal surface?
  - Charging of periodic structure?
  - Electronic structure - charge transfer?

1. B. P. Klein et al., *J. Phys. Chem. C,* 123, 2019, 29219-29230.
2. S. J. Hall, B. P. Klein and R. J. Maurer, arXiv:2112.00876.

FHI-aims
The ab initio materials simulation package

Charge transfer?

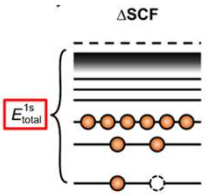


Gasphase Azulene

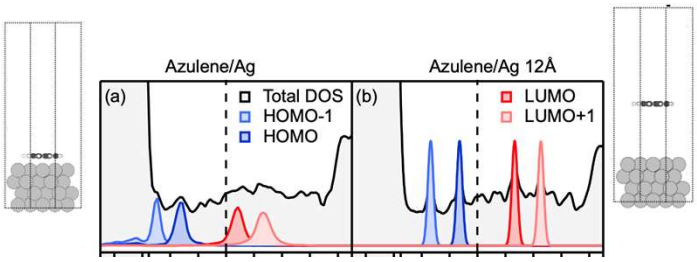
HOMO LUMO

S. J. Hall, B. P. Klein and R. J. Maurer, arXiv:2112.00876.

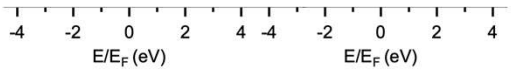
Spurious charge transfer!



ground-state DFT



core-hole excitation



Core-hole excitation in DFT introduces spurious charge transfer!

S. J. Hall, B. P. Klein and R. J. Maurer, arXiv:2112.00876.

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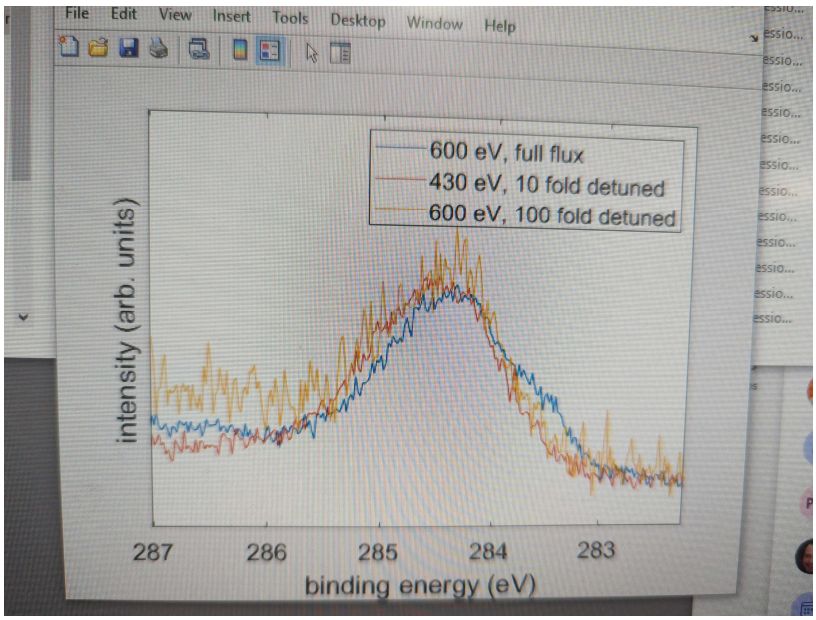
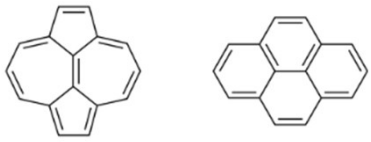
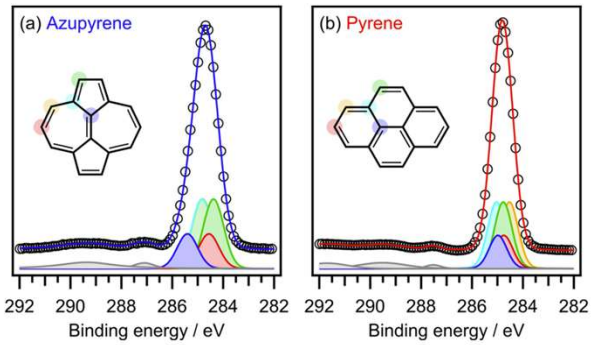
Sometimes it's not a shoulder, it's just beam damage



Azupyrene and Pyrene

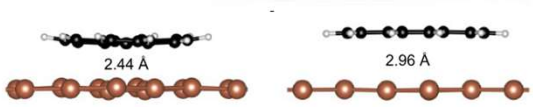


XPS

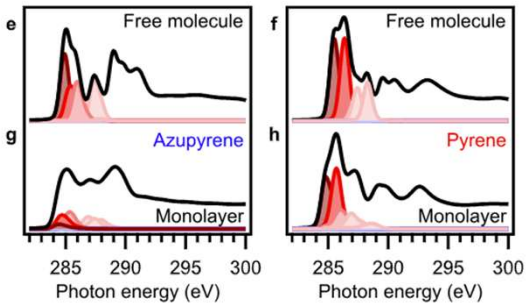


Klein et al., ChemPhysChem 22, 1065-1073 (2021)

@Cu(111)

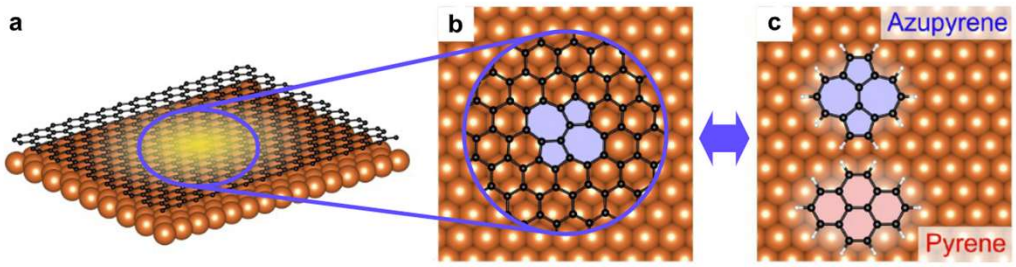


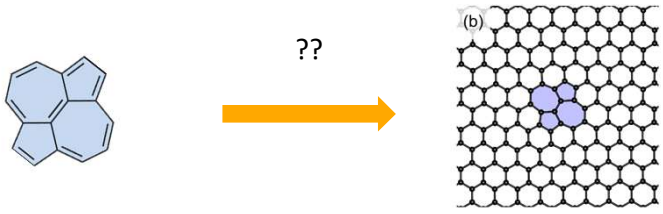
NEXAFS



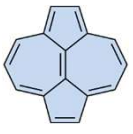
Klein et al., ACS Nano, 16, 8, 11979–11987 (2022)

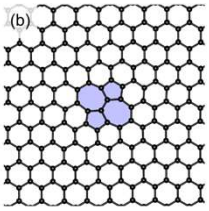
Azupyrene – a molecular model of a Stone-Wales defect





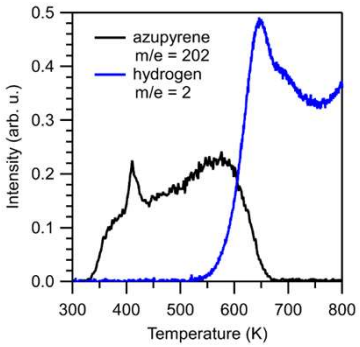
What is happening with azupyrene on Cu(111)





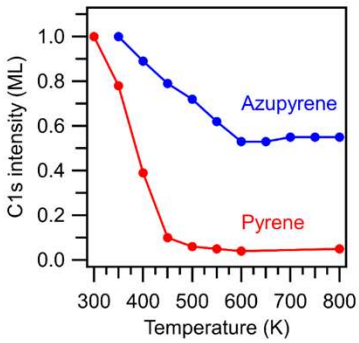
??????

TPD



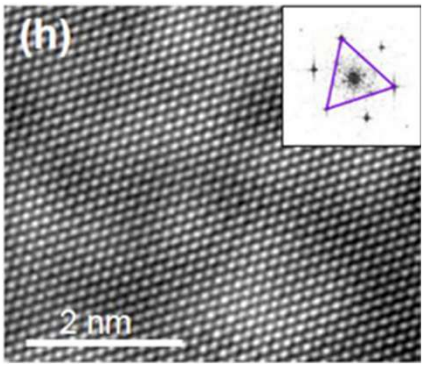
- Bond with the surface strong enough to enable dehydrogenative coupling
- But what is the result?

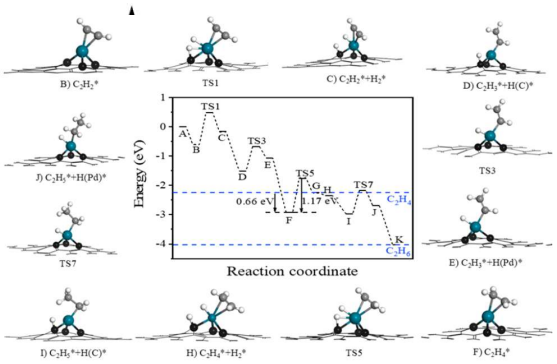
XPS



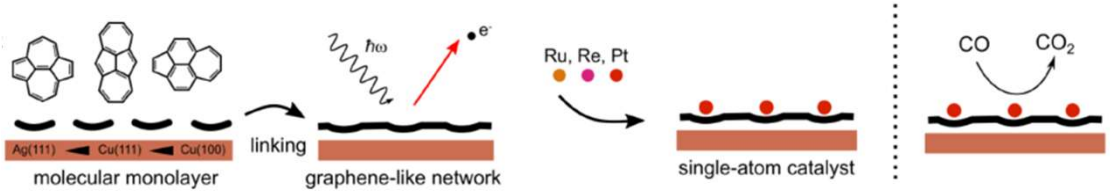
- Only partial desorption
- H_2 evolution

The Beauty of Imperfection: Topological Design of Defective Graphene

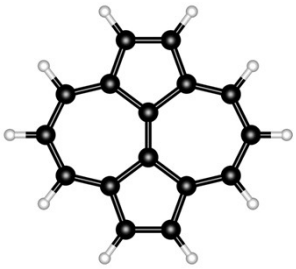




F. Huang, et al., J. Am. Chem. Soc., 2018, 140, 13142-13146



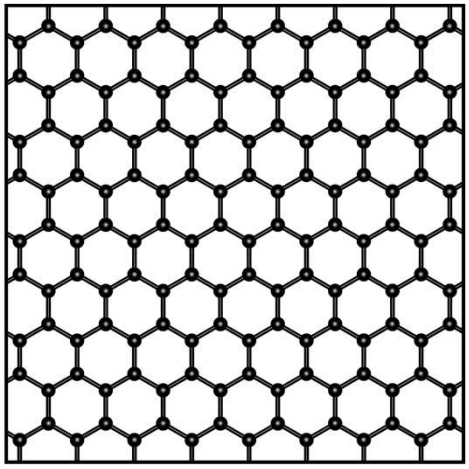
Growing defective graphene from azupyrene?



Azupyrene

??

High T deposition on Cu(111)



Benedikt Klein

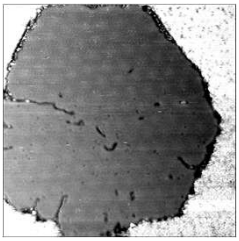
Matt Stoodley

David Duncan

Appl. Phys. Lett. **121**, 191603 (2022); doi: 10.1063/5.0122914

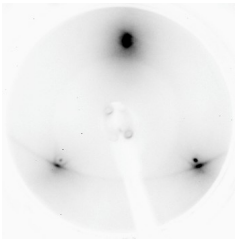
Proving graphene synthesis using azupyrene

1. Moire pattern visible in STM



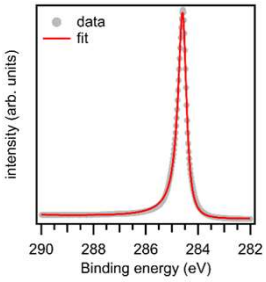
90×90 nm²

2. Rings in LEED

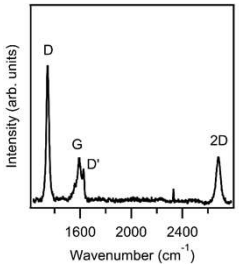


63 eV

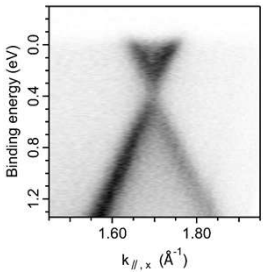
3. Sharp peak in C 1s XPS



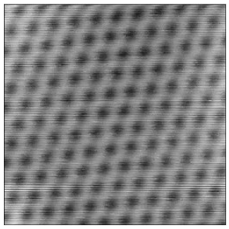
4. Specific Raman peaks



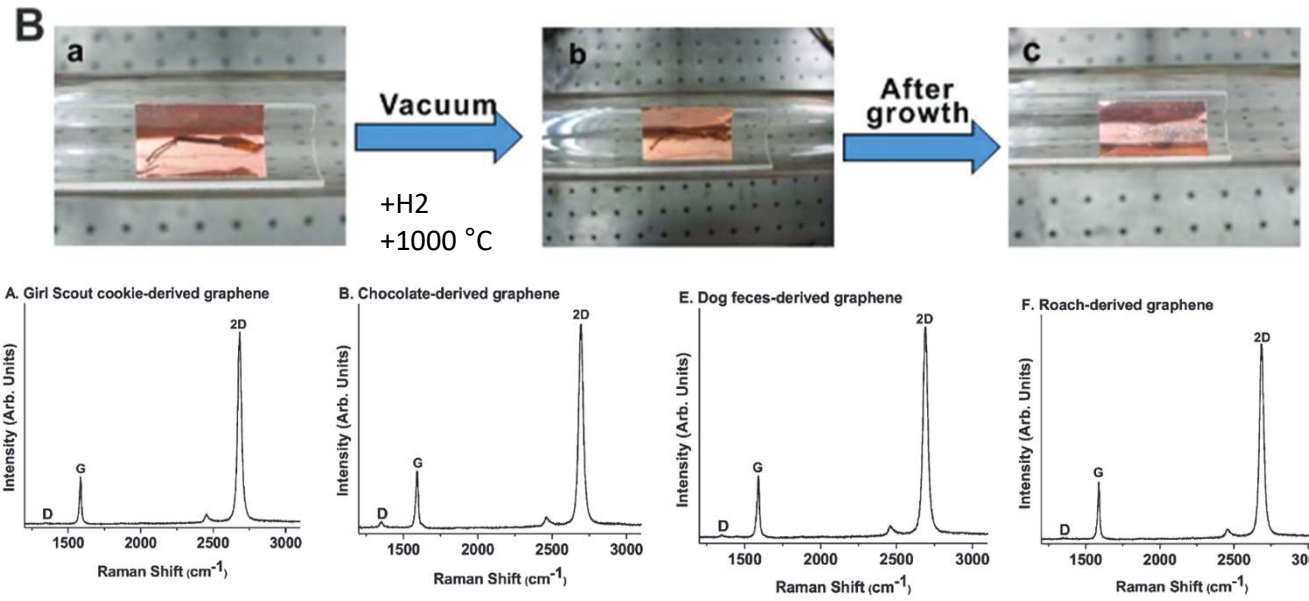
5. Dirac cone in ARPES



6. Atomic resolution, LT-STM

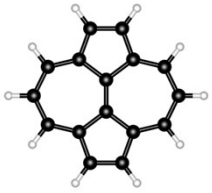


Is there anything that doesn't convert to graphene on copper?



Ruan, Sun, Peng, Tour, ACS Nano 2011, 5, 9, 7601–7607

Synthesis of defective graphene networks using

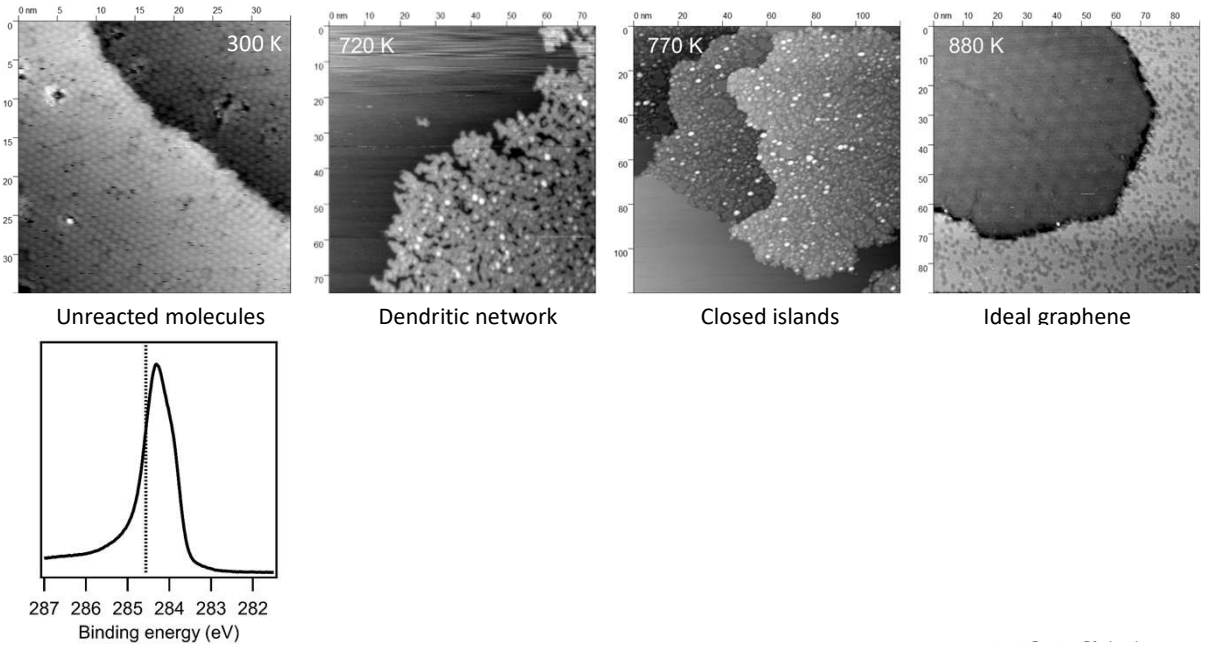


Continuous deposition onto Cu(111)
At elevated temperature

????

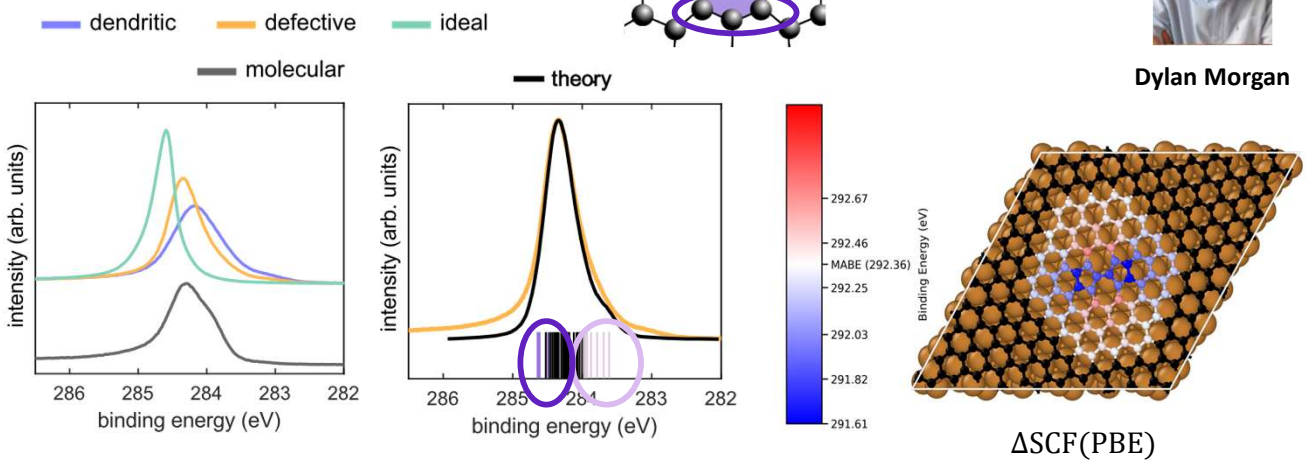
Room temperature STM images, taken in the SIL, DLS

Identify the graphene-like networks via HR-XPS



Taken at I09, hν = 430 eV

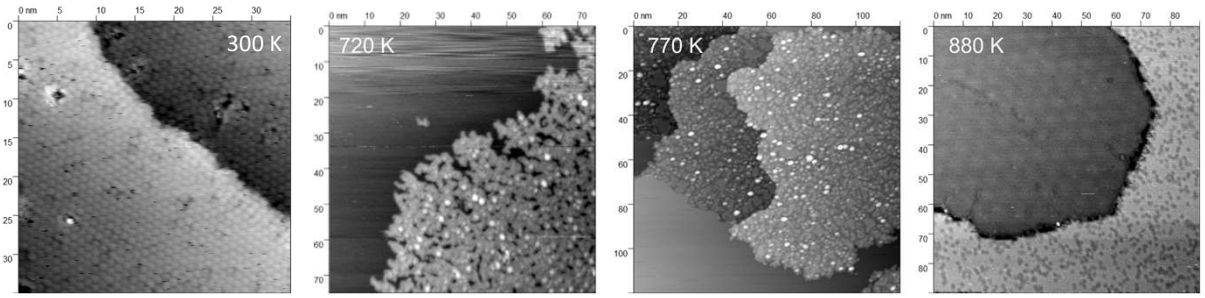
XPS – exp & theory



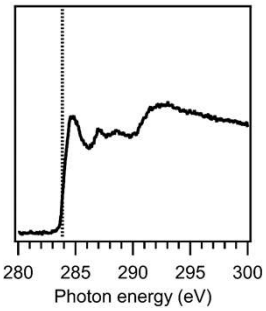
Dylan Morgan

B.P. Klein et al., Chemical Science 16 (41), 19403 (2025)

NEXAFS measurements of the graphene-like networks

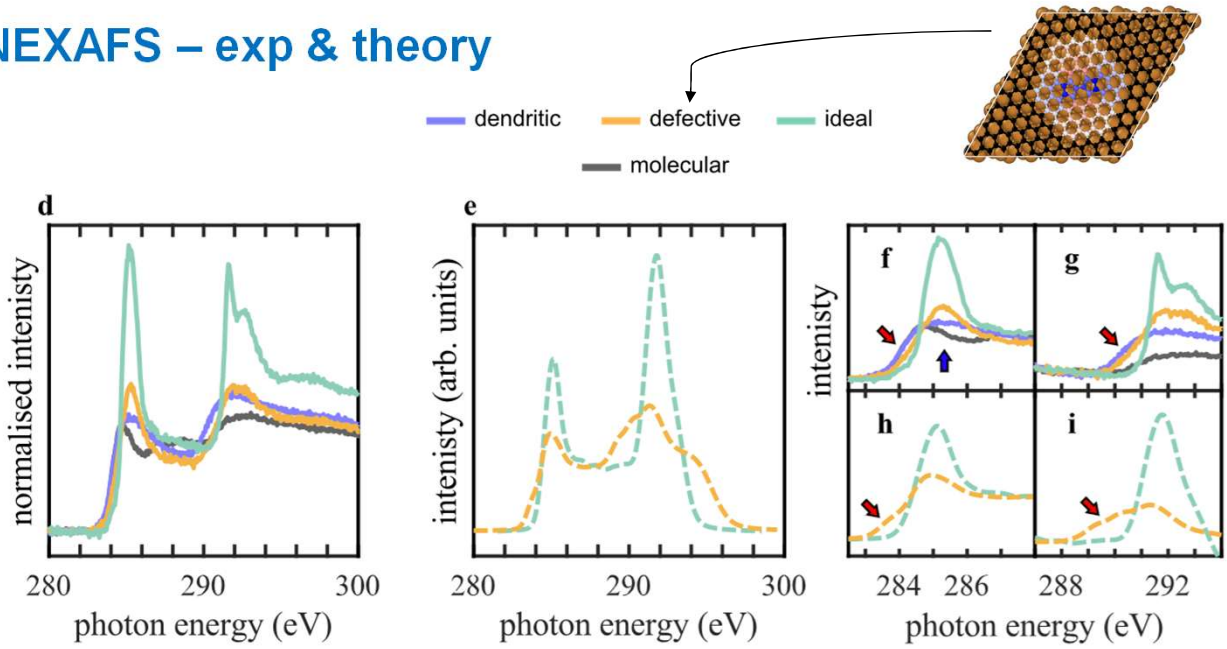


Unreacted molecules | Dendritic network | Closed islands | Ideal graphene



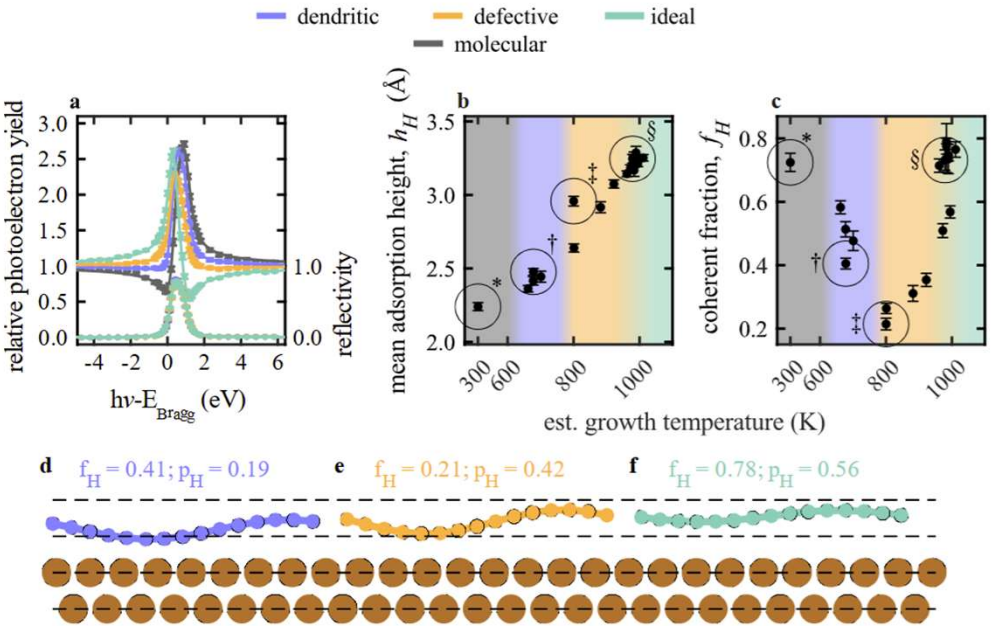
Taken at FlexPes beamline, MAX IV, Partial yield detection

NEXAFS – exp & theory



B.P. Klein et al., Chemical Science 16 (41), 19403 (2025)

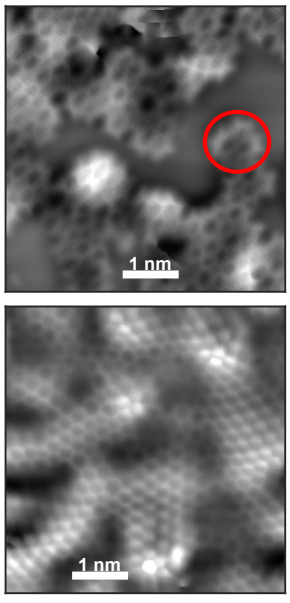
Quantitative Structure Determination – X-ray Standing Waves



Defect quantification: nc-AFM

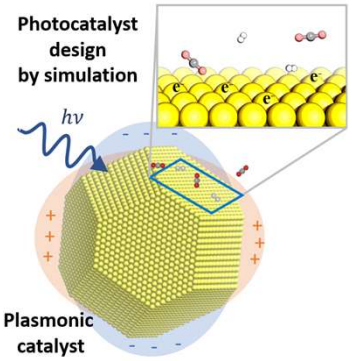
dendritic

defective



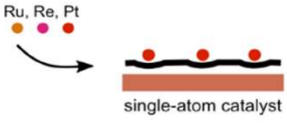
B.P. Klein et al., Chemical Science 16 (41), 19403 (2025)

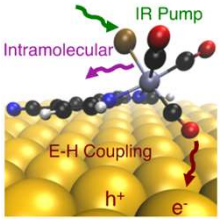
Computational Surface Science group

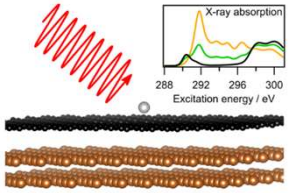


Ultrafast energy transfer & surface spectroscopy

Design of functional nanostructures







Thank you for your attention!