MCh rules

V.7.5 June 2025 +x
V.1.0 January 2007

Xxx: new
Xxx: revisitation as this does not work

Why do we need rules?

... to enable better science.[1]

We adhere to the Vancouver recommendations:

https://www.forskningsetikk.no/en/resources/the-research-ethics-library/legal-statutes-and-guidelines/the-vancouver-recommendations/

Mental health measures (1/4)

Grading system for responsibilities

- > 1 month after taking over a responsibility, the time used for this responsibility is monitored in hours/week by each PhD student (hours/weeks are averaged over at least 4 monitored weeks)
- Counted hours include:
  - Maintenance, repairing, introduction of machines
  - Service measurements with machines (excl. measurements for your research project)
  - Teaching and preparation time
  - Organization time, e.g. HiWi orga, PR, etc.
- The averaged hours/week (per responsibility) are sent to Marcus (including the list of monitored days, see excel template) and is basis for the discussion in next responsibility meeting
- Start of data collection in October 2022

Mental health measures (2/4)

- Every new PhD student may choose one mentor & mentor needs to agree (senior PhD student or postdoc)
  - Responsible person for HiWis will introduce new PhD student to mentoring system and mentoring should start within the two first months of the PhD
  - During the first year, they meet once a month (mentee should prepare topics (s)he likes to discuss; focus should be general challenges or limitations rather than deep scientific discussions)
  - Mentor can join (progress) meetings between mentee and JMS
- Every PhD student can participate in workshops offered by the RWTH Doctoral Academy, SFBs, etc.
  - Synchronize plans with jms

Mental health measures (2/3)

- Appraisal interviews with PhD students is organized once a year (after the planning meeting)
  - JMS gives PhD students feedback about their scientific and professional progress, addressing

    → scientific writing,

    → presentation skills,

    → research planning, and

    → soft skills

    in the form of generalized feedback that summarizes the feedback received over the year in a few sentences including 80-100% (salary) “average” benchmarking, including at least 2-3 positive and 2-3 improvable qualities

Mental health measures (4/4)

- PhD students give JMS anonymous feedback about 2-3 positive and 2-3 improvable factors of their PhD (before the planning meeting and the appraisal interview)
- Anonymous suggestion box (“Kummerkasten”)
  - If personal discussions with JMS and/or mentor are not considered to be helpful, PhD students can submit anonymously urgent worries, challenges (preferably with constructive change requests) to the suggestion box
  - PhD students are protected in their anonymity

Safety: New Hiwi's & Researchers

- The following lab safety course(s) are required prior to doing ANY work in the lab:
  1. Mr. Conrad, electrical safety issues
  2. Mr. Momma, general safety issues
  3. Dr. Fečík dangerous chemicals / substances

- ALL electrical modifications of experiments need to be approved by Mr. Conrad and Dr. Mraz

- The following lab technical course(s) are required prior to doing ANY work in the lab:
  1. Mr. Momma, mechanical engineering
  2. Dr. Mraz vactec engineering

Before starting your Ph.D. or within the first 6 months the course MCh DNA has to be completed

All documents…

contain:

Your name

The date

Page numbers

In word: Use Helvetica 12, double spaced

Research planning: RQs

- Define 3+ RQs with jms – here the research is conceived
- **Over time the RQs will be refined** taking new knowledge (from you and others) into account

- Describe each RQ and how you seek to answer it in <250 words

- Start **ALL internal** research presentations with the RQ(s) and your time axis

- The answer to a RQ is given in our publication

- Save RQ.doc in sciebo in your folder RQs, use manuscript file name syntax

- Add the RQ on the first page of the manuscript

Example RQ

RQ1: Quantification of the fraction of hybridised bonds in metallic glasses

Schnabel et al. proposed a low overall fraction of hybridised bonds as a measure of damage tolerance in metallic glasses by comparison of Au-, Co-, Cu-, Pt- and Pd-based metallic glasses [1]. Thus, the design of tough metallic glasses is favoured by a minimised fraction of hybridised bonds. Following this design proposal, a Pd-based metallic glass has been designed and synthesised that is too tough to investigate by fracture mechanics (bending). To critically appraise this design proposal and generate a design criterion, the electronic structure of this metallic Pd-based metallic glasses will be compared to the electronic structure of glasses with fracture toughness and yield strength known from literature [2]. The fraction of hybridised bonds will be quantified by the Crystal Orbital Overlap Population to establish a relationship between the fraction of hybridised bonds and fracture toughness.

The aim of this work is to quantify the fraction of hybridized bonds and relate it to the toughness of metallic glasses in order to critically appraise the design proposal for tough metallic glasses.

[1] Schnabel et al., *Electronic hybridisation implications for the damage tolerance of thin film metallic glasses*, Scientific Reports **6** 36556 (2016)

[2] Demetriou et al., *A damage-tolerant glass,* Nature Materials **10** 123-128 (2011)

Planning meeting

- At least one planning meeting per year
- All Ph.D. students have an external advisor (Leoben, Wien, Thun)
- At least one meeting with external advisor per year
- Use presentation template for MCh planning in appendix
- Update RQ file at least 14 days before the planning meeting and bring it to the meeting

Publications (1)

Mean what you say and say what you mean
& assume responsibility for **YOUR** story

Compile manuscript skeleton:

- 1st page: RQ
- 1st page: the story in 5+1 sentences:
  - 1. hypothesis (1)
  - 2. experiments (1) + calculations (1)
  - 4. observation (1)
  - **5. explanation (2)**
- 2nd page: title, authors, abstract & target journal
- subsequent pages with all figures with a concise description of the key data

→ Once we agree on the skeleton, please draft the full paper, see template.

Publications (2)

Format, see template:

- Helvetica 12, double
- spaced, justified text
- Single page

- Page number / file name on every page centered at page bottom page number

- Print out in color

- Include figures, tables and captions in the text where you discuss them

- Format in line with the figure templates enclosed NOT NEW BUT OFTEN IGNORED

- Check spelling

Publications (3)

- Upload manuscript & send by email to jms:
  - DOC file with file name syntax: 2019_05_25_xy_#1_V1.doc & (without figures)
  - Use track changes with “show all revision in-line”
  - PDF file with file name syntax: 2019_05_25_xy_#1.pdf (without figures)
  - Figures only PDF: F_2019_05_25_xy_#1.pdf
  - Comments only PDF: F_2019_05_25_xy_#1.pdf

  → xy=your initials; #1=manuscript #1; V1=Version1
- Upload pdf’s of all references to sciebo
  - File name syntax: Gall_PRB_2000.PDF
- Put unstapled printout with date stamp in blue plastic cover in jms mail folder.
- Include previous versions.

Publications (4)

- Mark changes with track changes
- Implement my changes
- Implement changes of the coauthors from other groups
- Do not delete my comments
- If you don't like these suggested changes implement them anyway and add your comment

Figure templates 1

- Figure format: Use color

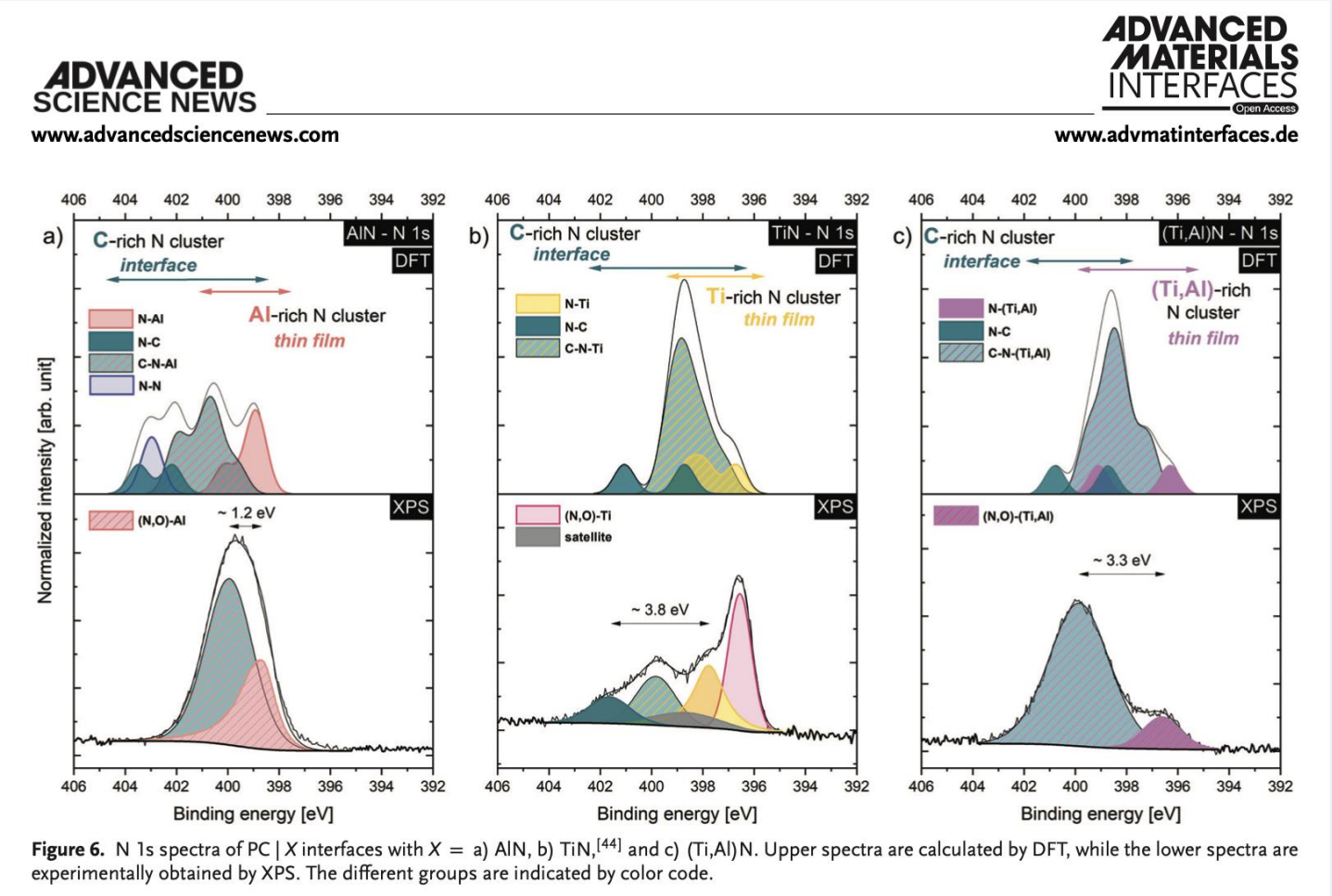


Figure 6. N 1s spectra of PC | *X* interfaces with *X* = a) AlN, b) TiN,[44] and c) (Ti,Al)N. Upper spectra are calculated by DFT, while the lower spectra are experimentally obtained by XPS. The different groups are indicated by color code.

See, Patterer et al. Advanced Materials Interfaces 2023

Figure templates 2

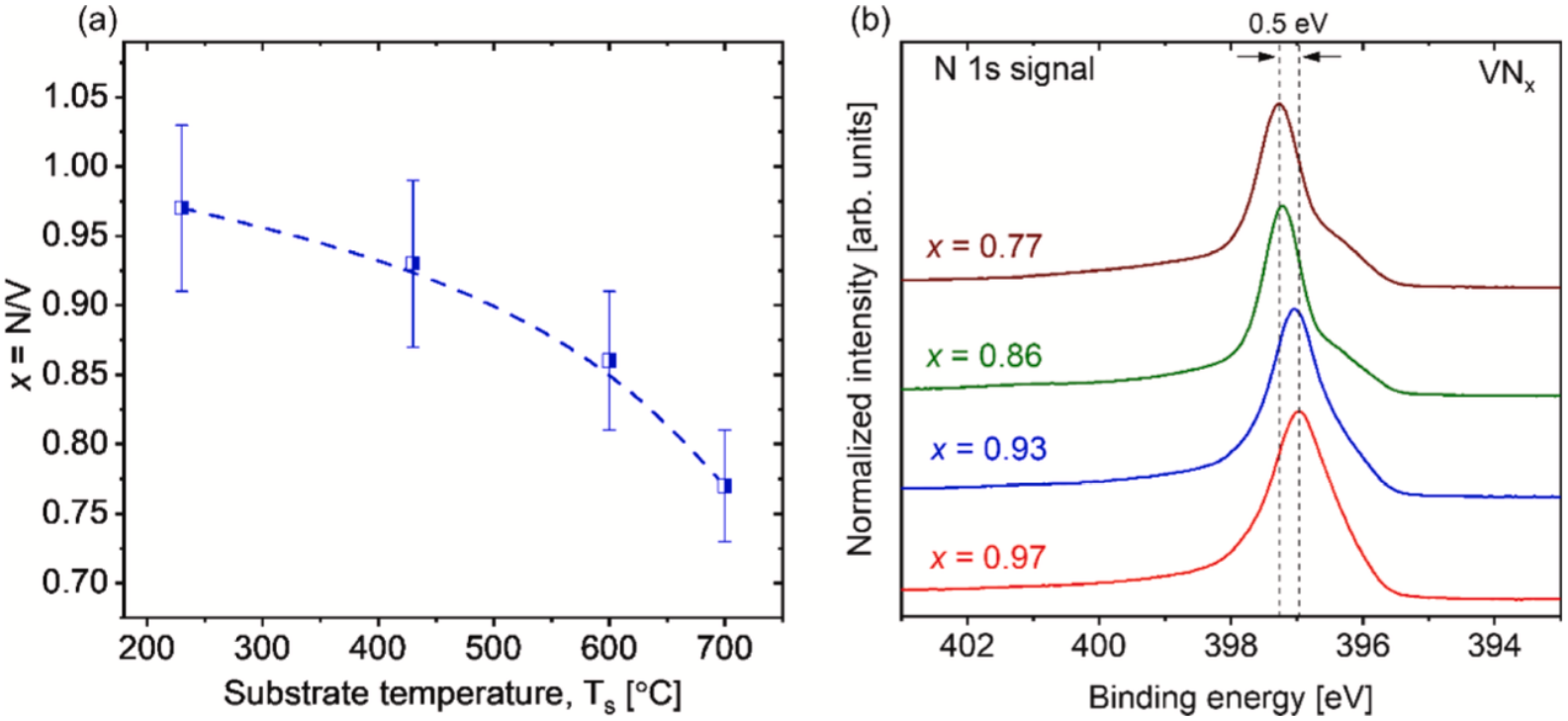


Fig. 5. (a) N/V ratio x of VN_x/MgO(001) thin films deposited by DCMS as a function of substrate temperature determined by TOF-ERDA. (b) XPS N 1s spectra of (a) VN_x/MgO(001) with respect to N/V ratio x.

See, Karimi et al. *Acta Materialia 255 (2023) 119078*

Figure templates 3

- Figure format: Use color

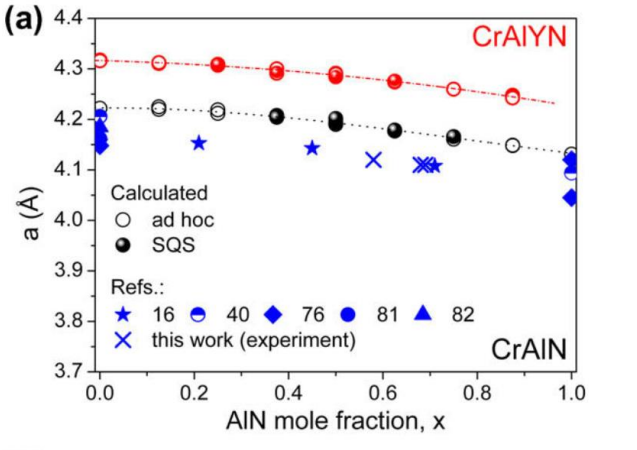


Fig. 6. Ab initio calculated (a) lattice parameters and (b) bulk moduli as a function of the AlN mole fraction x for fcc (B1) $Cr_{1-x}Al_xN$ and fcc (B1) $Cr_{0.875-x}Al_xY_{0.125}N$ as obtained from ad hoc and *SQS* supercells. Values reported and experimentally obtained in the literature are added for comparison.

- See Rovere_ActaMat_2010

Figure templates 3

- Figure format: XRD

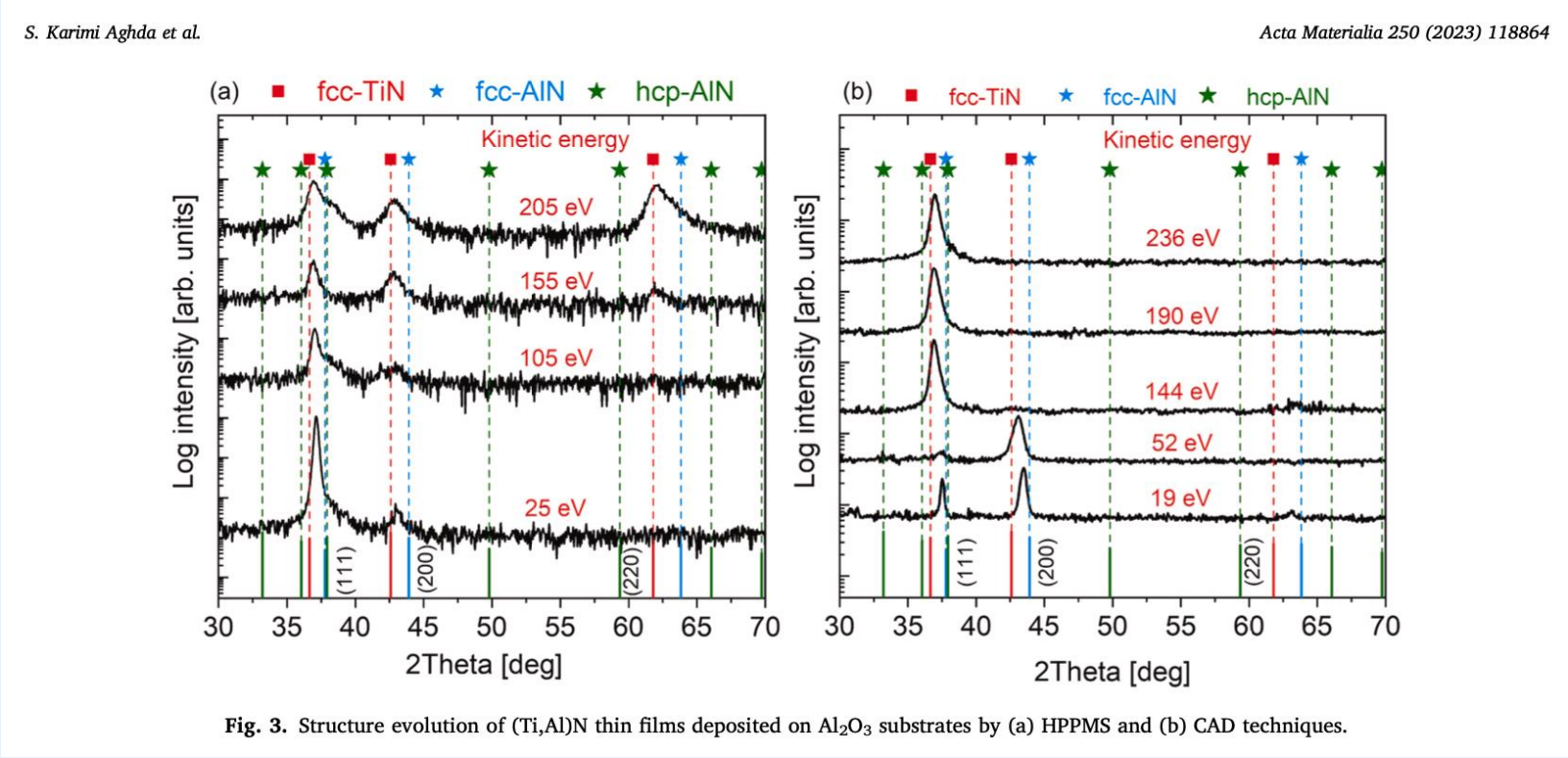


Fig. 3. Structure evolution of (Ti,Al)N thin films deposited on Al_2O_3 substrates by (a) HPPMS and (b) CAD techniques.

- See Karimi et al

Publications (6)

- Send PDF of **published** manuscript to Dr. S. Münstermann, cc: Strauch, jms
- Upload the final publication with full bibliographic details at RWTH publications (https://publications.rwth-aachen.de) so that the paper appears on our homepage. Mh can help in case of questions
- Upload to ONLY open access pubs @ researchgate
- Do NOT upload NON open access pubs @ researchgate
- Create a RWTH Personal Data Set @ https://www.ub.rwth-aachen.de/go/id/iihb

Manuscripts with external partners

- Only one version with comments from MCh
- Jms approves before sending the MCh corrections to the external partner

Data management

- from the contract: every member of MCh is responsible for their own data and that they are properly stored and managed

- after publishing a paper:
  - in your Exchange folder, create a directory YYYY_MM_DD_rq#
    - rq# = research question no., YYYY_MM_DD = date the article was accepted for publishing
  - store all your data relevant to the published article in this directory

- before leaving MCh for good, make sure all your data are properly uploaded and stored
  - experimentalists:
    - all your electronic data need to be stored in your Exchange folder with proper naming
    - store samples (marked with correct ID) in dedicated sample storage cabinet!
  - theoreticians:
    - all your important and relevant data need to be moved from HPC to MCh local file system (Exchange)
    - relevant data: inputs, outputs, pseudopotentials, models, etc. (i.e. no particularly large files)
  - no need to re-upload data of published articles (as long as the previous steps done correctly)
  - make sure that your colleagues have access to your samples and your data!

- curent RDM solution: Kadi4Mat (under construction) (administrator: Michal Fečík)

Ph.D. thesis (1)

- We agree on goals and strategy (RQ)
- Duration: 48 months incl. teaching + service analysis + course admin. + examination board equipment responsibility, etc.
- Half time research presentation for MCh and your external examiner 30min:
  What have you understood in the last 24 months?
  What do you still need to understand?
- Main authored publications: Min. 2 accepted as thesis is handed in and min. (3-$n_{accepted}$) submitted
- Max. length: 120 pages, font Helvetica 12 double spaced

Ph.D. thesis (2)

- Grades:
  "mit Auszeichnung" = "with distinction" **Fak.V rule** = MCh rule: **Only 5-10% of all dissertations**
  "sehr gut" = "very good"
  "gut" = "good"
  "genügend" = "sufficient"

Ph.D. thesis (3): list of content

MSc and BSc thesis, mini thesis, Hauptseminar

- The advisor has to announce all thesis projects BEFORE START to Dr. Münstermann
- The paper work – which is different for different study courses has to be filed at least in copy with Dr. Münstermann

Thesis length

- Ph.D. max. 120 pages
- Master/Dipl. max. 60 pages
- BSc thesis max. 30 pages
- Studienarbeit/Internship max. 30 pages

KEEP IT SHORT AND SWEET!

Iterations…

... always hand in ***the previous version and mark the changes***!

Scientific talks

- Define goal of the talk
- Consider your audience and define content
- Discuss goal & content with jms (and others…)

- **Use MCh template (this PPT file)**
- ≥14 days before the talk send email + printout with stamp to jms mail folder

Project meetings, SFB etc.

- Define goal of the talk (consider political components)
- Define the scientific goal
- Consider your audience and define content
- Discuss goal & content with jms

- **Use MCh template (from this presentation)**
- ≥14 days before the talk send email + printout with stamp to jms mail folder

Wednesday talk

- 15 min. + discussion (approx. 15 slides)
  - standard conference talk template
  - Internal talk therefore start with RQ or RQs
- Motivation for presentations:
  - updating the group on progress & challenges
  - method section if relevant
  - information transfer (both ways)

Journal Club only for PhD students & jms

- All PhD students present 15 min. + discussion (approx. 15 slides)
  - standard conference talk template
- Motivation for presentations:
  - Share elegant and efficient research strategies
  - Elegant experiments
  - Elegant interpretations
  - Unconventional “horizon extending” strategies, methods, interpretations
  - Once a year you can give a “wild card” talk: This talk is outside of the scope of regular journal club presentations. The only criterium for this talk is that the presenter likes the topic and would like to share it within journal club.

Teaching

- Teach the exercises
- Teach when I am travelling
- Compile the draft-exam (talk to jms **before**)
- Correct the exam (group effort):
  - Show me the 5 best exams and the ones that did not pass by 2 and less points
  - Hand in the grading 'instruction'

Post-exam review: In case of conflict – I decide – take a written statement of the student

Responsibility meetings

- Marcus moderates the meeting.
- Goal is to share the time required for teaching incl. Labs, external analysis, equipment responsibility etc. equally within MCh.
- Marcus will call a new meeting if you think the responsibilities are not shared equally.
- Equipment responsibility includes education & drivers license transfer
- Manual + error & repair history

Meetings with jms

- Please inform me about all the cool things that you have understood or measured or calculated
- Please inform me about everything that frustrates you and impedes your progress
- Define meeting objective & keep it short and sweet
- Start with the RQ that you are addressing

Hiwis

- Hiwi = potential Ph.D. student!
- Introduce the hiwi to ALL group members
- You are responsible for the hiwi
- Introduce her/him to the rules
- You are responsible for the hiwi
- Communicate your expectations
- Check if the hiwi acts responsibly

Hiwi tasks

- **Science**
- Support of general MCh activities*

  * for example:

    copying, exam support, moving stuff, delivering stuff, etc.

Travel

- Submit travel request BEFORE your trip
- Plan travel +1 year ahead and discuss your plans with me
- Financial planning with sm and me
- Don’t buy your own ticket without agreement from sm
- Travel reimbursement Fr. Strauch

Vacation

- Submit vacation request BEFORE vacation

Ph.D. Student Salary

- Start with 60% salary €€€
- After 6 months +20% €€€€
- 1st paper draft accepted jms +20% €€€€€

The END

Appendix

- Planning meeting template
- Group presentation template

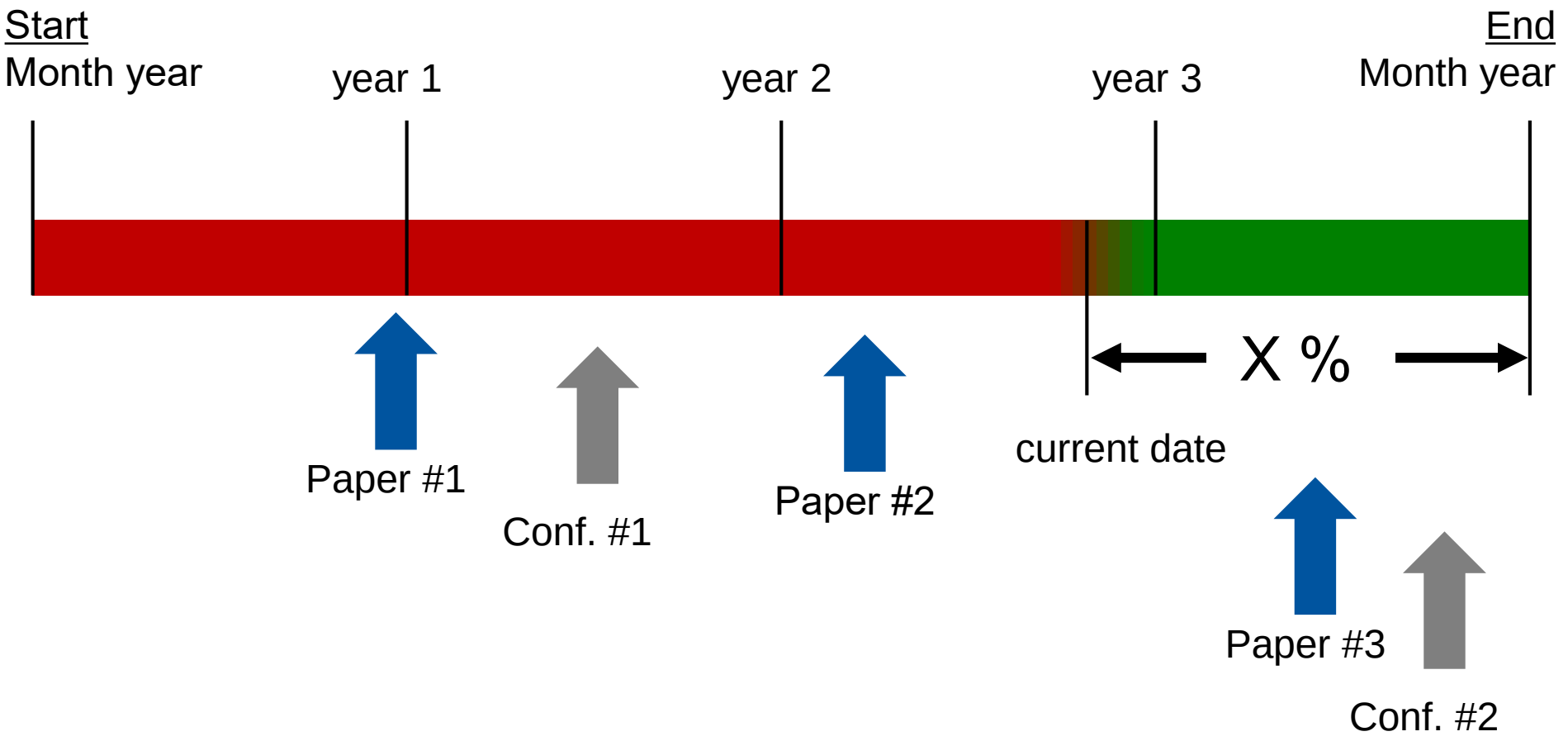
Planning meeting

Name

Month year

MATERIALS CHEMISTRY | RWTH AACHEN UNIVERSITY

Timeline: PhD



Research questions/topics

1 Title 1

➢ **Current status // next step** 100% done

2 Title 2

➢ **Current status // next step** 100% done

3 Title 3

➢ **Current status // next step** 20% done

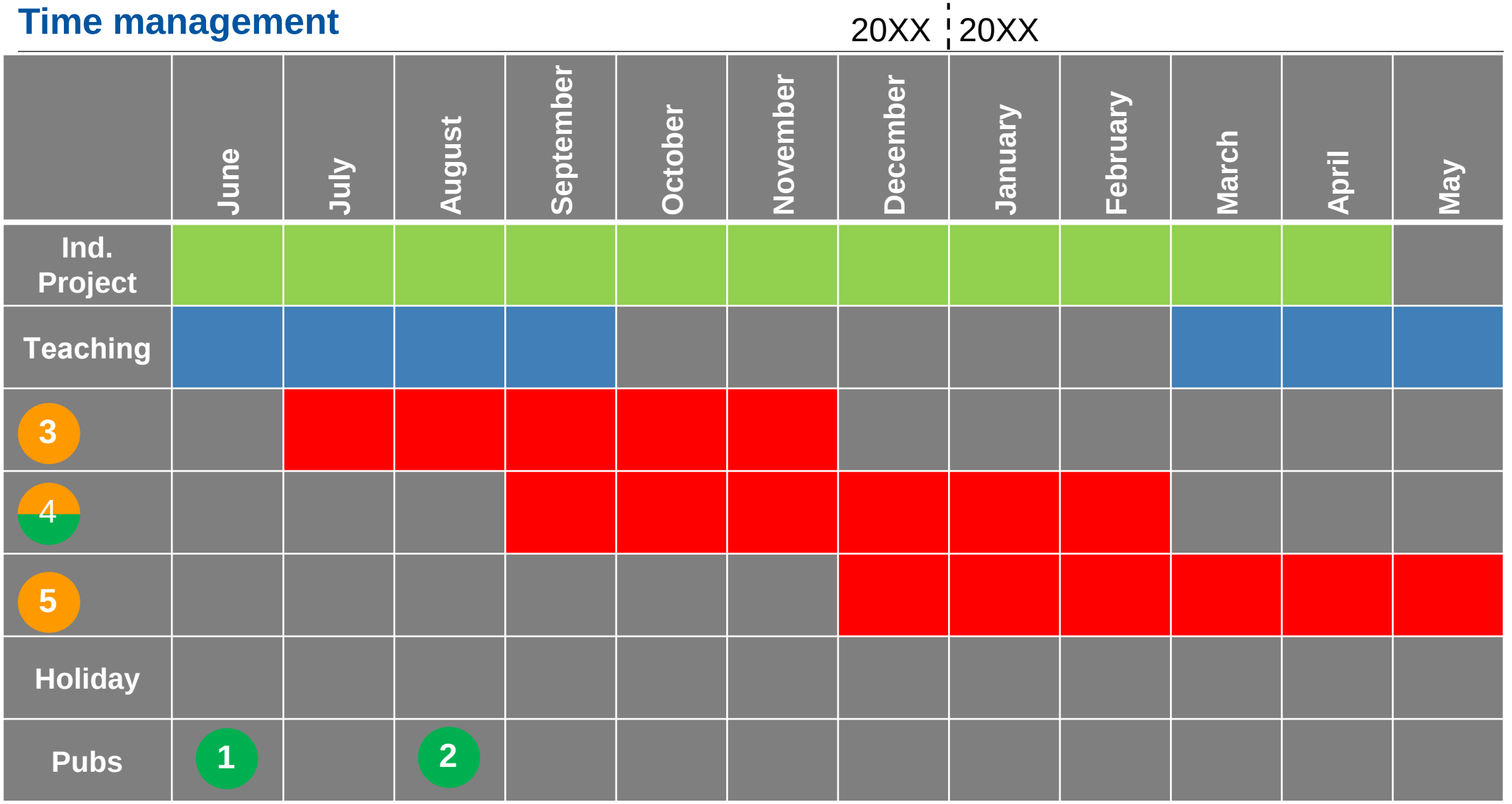
.....

3 Research questions/topics

RQ aim: …

XXXX done Next: XXXX

Time management



MATERIALS CHEMISTRY | RWTH AACHEN UNIVERSITY

Limiting factors

1. xxxxx
2. xxxxx
3. xxxxx
4. xxxxx

Bond formation at PC | X interfaces studied by DFT & XPS

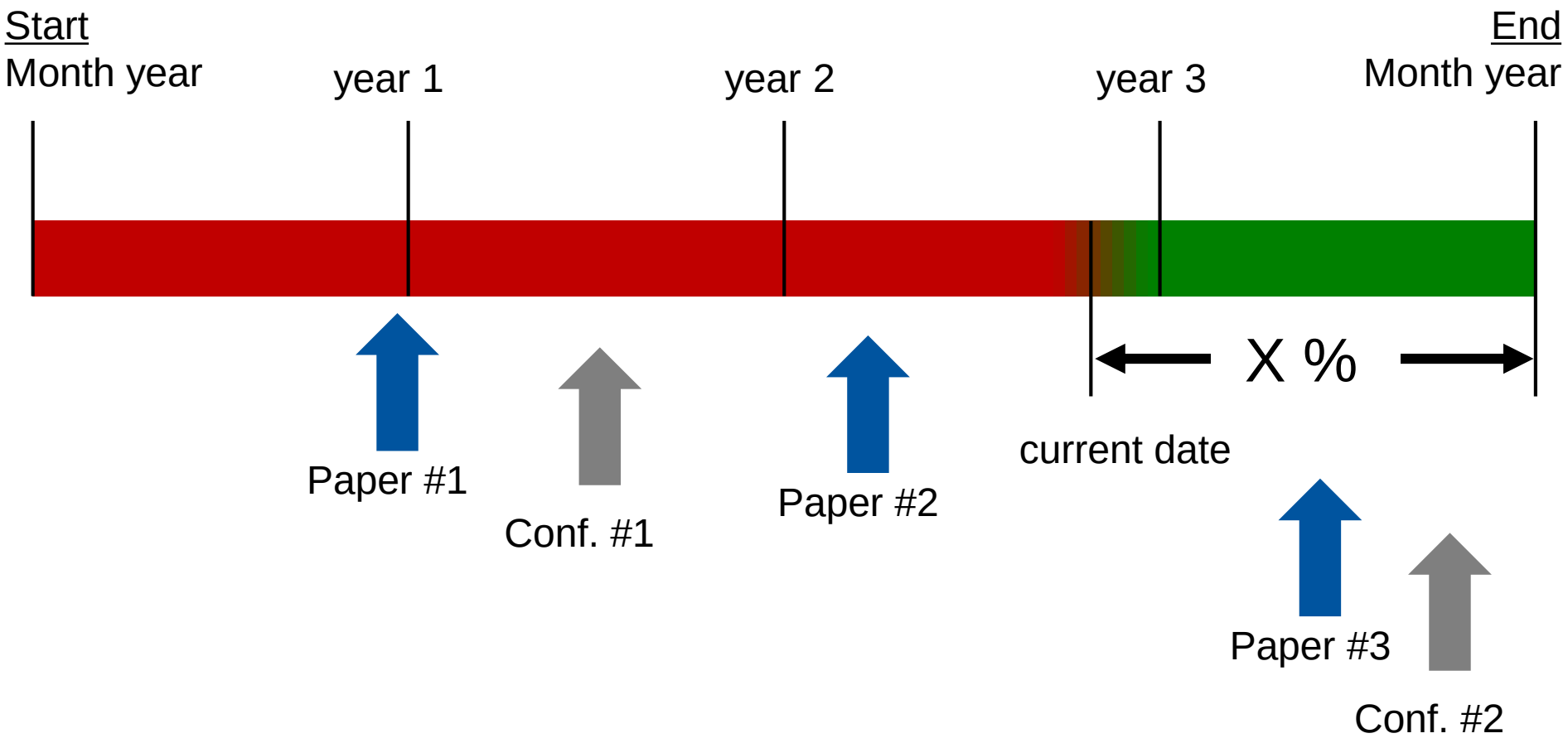
(X = Ti, Al, TiAl, TiN, AlN, TiAlN, TiO_2, Al_2O_3, (Ti,Al)O)

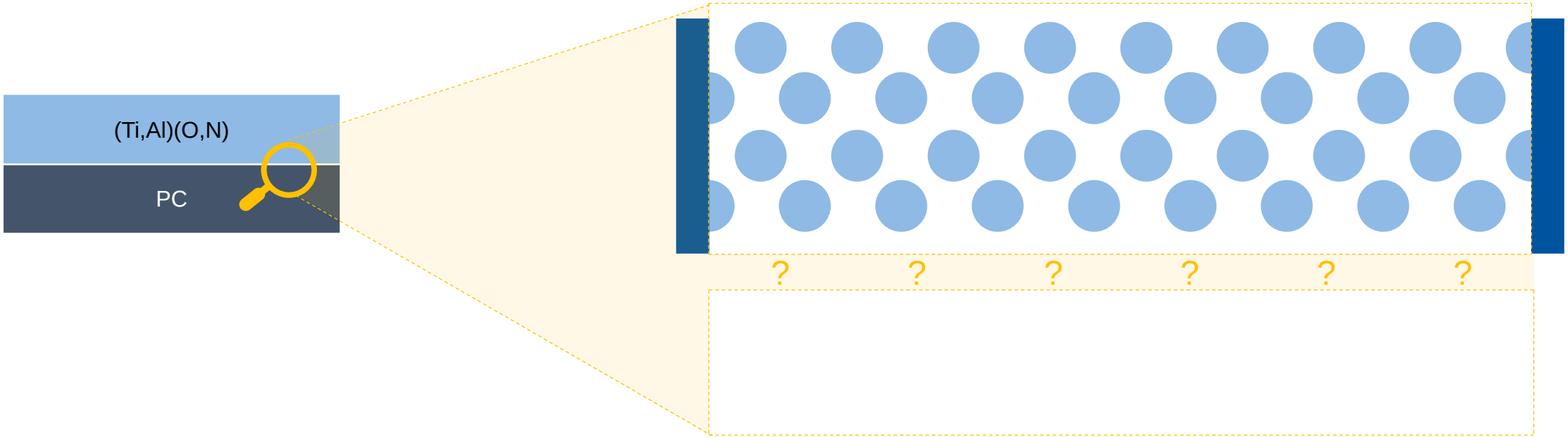
Wednesday talk – February 08, 2023

Lena Patterer

MATERIALS CHEMISTRY | RWTH AACHEN UNIVERSITY

Timeline: PhD / post doc





RQ’#?:

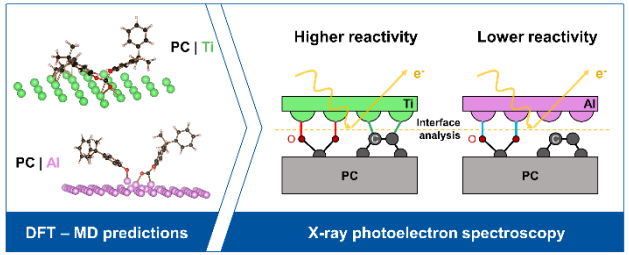
What bonds define the interface?

Context: Overview of projects on the interfacial bond formation with PC

Paper

Bond formation at polycarbonate | X interfaces (X = Ti, Al, TiAl) probed by X-ray photoelectron spectroscopy and density functional theory molecular dynamics simulations

Lena Patterer*, Pavel Ondracka, Dimitri Bogdanovski, Leonie Jende, Stephan Prünte, Stanislav Mráz, Soheil Karimi Aghda, Bastian Stelzer, Markus Momma, Jochen M. Schneider



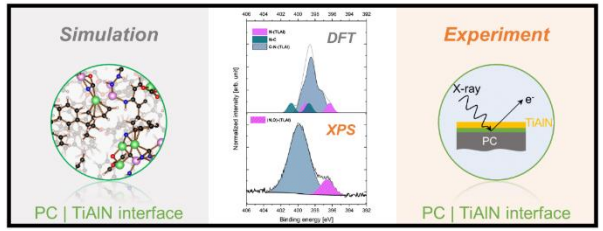
Metal

Ti, Al, TiAl

Manuscript

Correlative theoretical and experimental study of the PC | X interfacial bond formation (X = TiN, AlN, TiAlN) during DC magnetron sputtering

Lena Patterer*, Pavel Ondračka, Dimitri Bogdanovski, Stanislav Mráz, Soheil Karimi Aghda, Peter Pöllmann, Yu-Ping Chien, Jochen M. Schneider



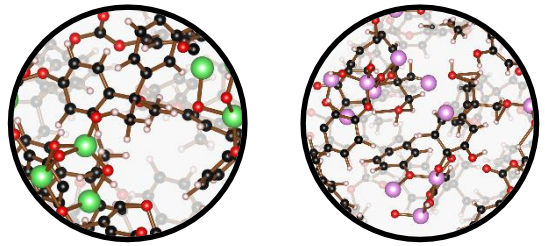
Metal nitride

TiN, AlN, TiAlN

Analysis of data

Theoretical and experimental bond formation at polycarbonate | X interfaces (X = TiO_2, Al_2O_3, (Ti,Al)O)

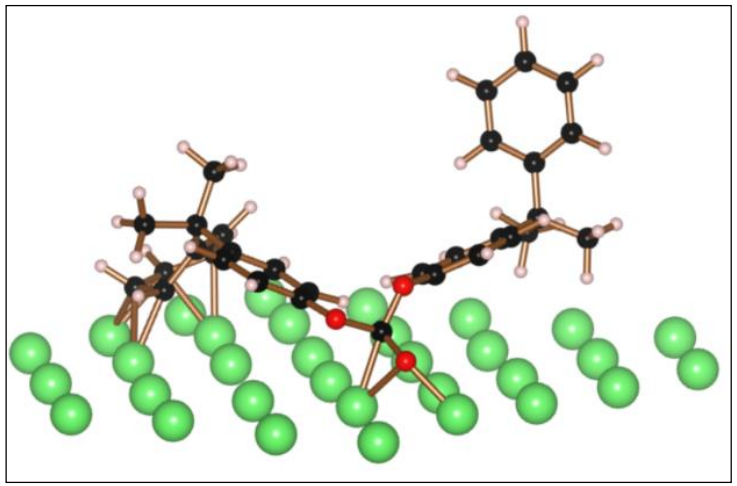
Lena Patterer[1]*, Pavel Ondračka[2], Dimitri Bogdanovski[1], Stanislav Mráz[1], Soheil Karimi Aghda[1], Jochen M. Schneider[1]



Metal oxide

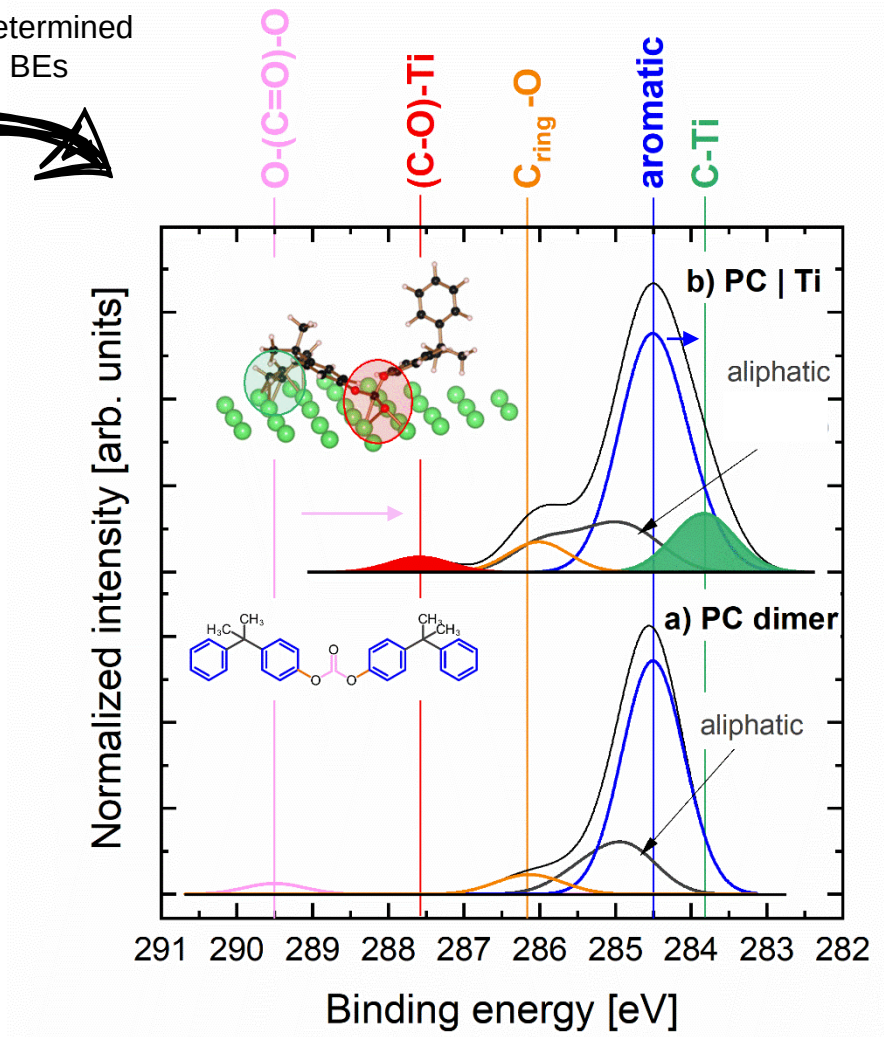
TiO_2, Al_2O_3, (Ti,Al)O

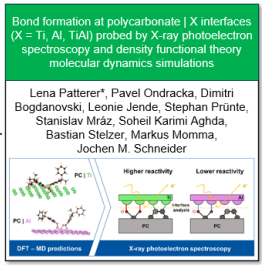
Binding energies for interacting PC dimer are calculated



Selected configuration of MD simulation

Theoretically determined broadened BEs





Momma, K.; Izumi, F. *J. Appl. Crystallogr.* **2011**, *44* (6), 1272–1276

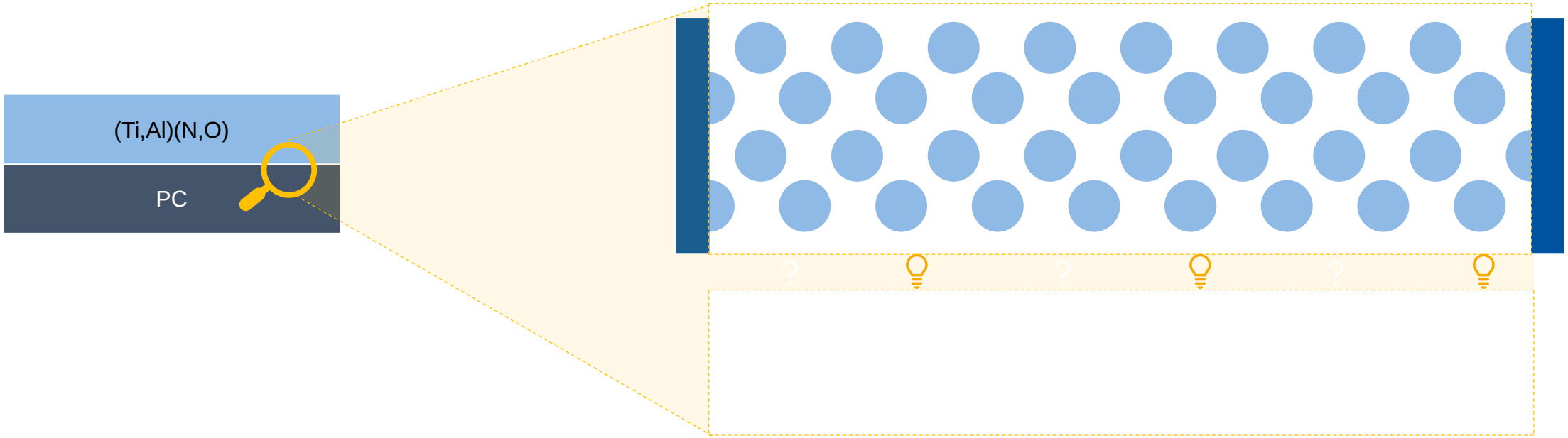
… more results

Lesson(s) learnt…

Theoretical and experimental bond formation at polycarbonate | X interfaces

(X = Ti, Al, TiAl, TiN, AlN, (Ti,Al)N, TiO_2, Al_2O_3, (Ti,Al)O)

- Ti, O and N are very reactive and form interfacial C-Ti, C-O-Ti, C-N, C-O bonds
- Al selectively reacts only with C-N and C-O groups
- C-N and C-O are strongest bonds at the interface
- The high reactivity of Ti is preferential for the metallic system, whereas for the nitride and oxide system less strong C-N and C-O bonds are formed



Thank you

for your attention!

Backup