UPPSALA UNIVERSITET

TECHNISCHE UNIVERSITÄT WIEN

Aalto University School of Science

EUROfusion Horizon Europe
(2021-2023)

ENABLING RESEARCH PROJECT

Electronic interactions of slow ions and their influence on defect formation & sputter yields for plasma facing components

Kick-off Meeting

https://wiki.euro-fusion.org/wiki/Project_No5

https://indico.euro-fusion.org/category/305/

Agenda

- Recap our working-packages, planned major tasks, expected deliverable and pm commitments
- Provide some information received from the ENR PMU (project life cycle, reporting, communications, etc).
- Discuss some formal arrangements, e.g., the official project starting date (for 3 years project – our case – **1st of July 2021 as latest**).
- Possible adjustments (per each calendar year) on the tasks according to our initial proposal.
- Open discussions (shared slides, etc)

Objectives & outcomes

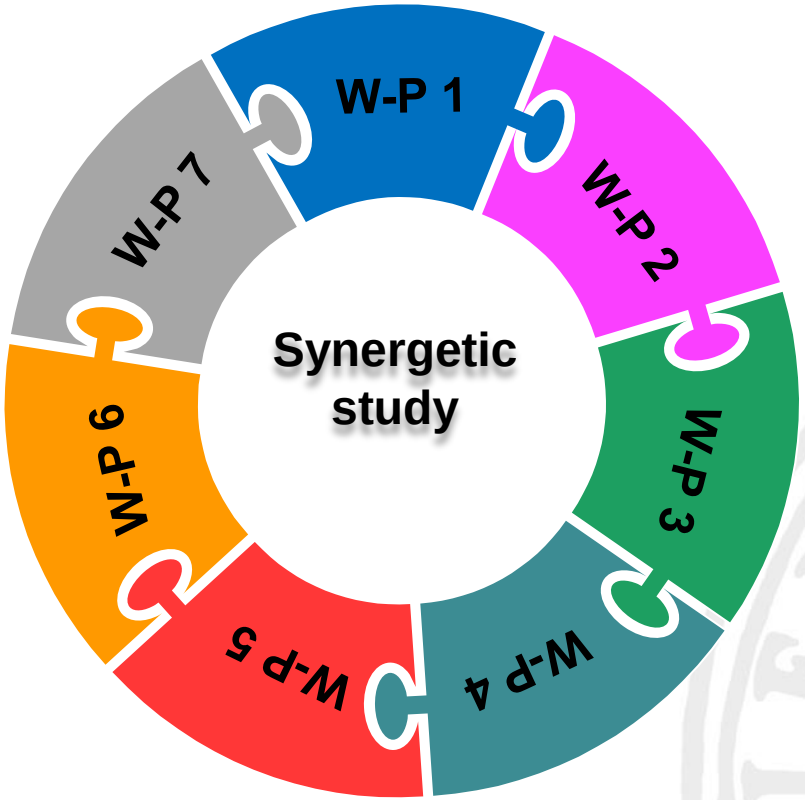
1. Experimentally deduce electronic energy loss of light ions (^{1,2}H, ^{4}He) in Fe, W and EUROFER at E << 100-200 keV.

2. Experimentally deduce short-range repulsive potentials for light ions (^{1,2}H, ^{4}He) in Fe and W at as low energies as possible.

3. Use (1) and (2) to benchmark advanced BCA-based codes (SDTrimSP & Tri3dyn): experimental sputtering yield results will be modelled using (1) and (2) as input data.

4. Computational investigation: real-time TD-DFT of electronic stopping power of light ions in Fe, W and EUROFER; MD simulations of sputtering from complex surfaces to check accuracy of the models; compare BCA and MD models to evaluate limitations in the low velocity regime.

Working-packages



Working-packages

General management

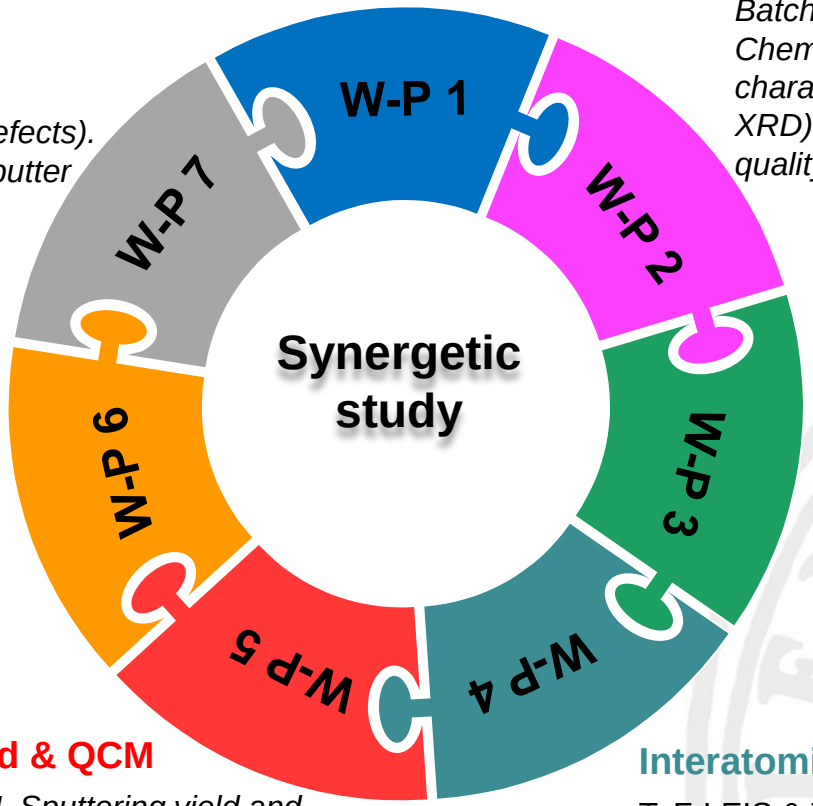
Kick-off meeting
Task coordination
Annual meetings (2)
Final meeting & reports

Computational modeling

TDDFT simulations of electronic stopping power of W, Fe and EUROFER-like (samples w/wo defects). MDRANGE: ion implantation & sputter yield (input: electronic stopping)

Sample preparation

Batches of Fe, W and EUROFER. Chemical and morphological characterization (e.g., AFM, SEM, XRD). Distribution and routinely quality control (ex-situ and in-situ).



Ion-irradiation experiments

Define irradiation conditions. Ex-situ and in-situ ion irradiation experiments on Fe, W and EUROFER @ UU and TU. Samples to be reused in W-Ps 3,4,5

Electronic energy loss meas.

Experimental stopping cross section of pristine Fe, W and EUROFER. For each sample @ keV and sub-keV regime. Compare experimental results between pristine & damaged

Sputtering yield & QCM

QCM set-up at UU. Sputtering yield and angular distributions of pristine Fe, W and EUROFER samples (@ TU and @ UU up to some extend). BCA-based simulations (SDTrimSP).

Interatomic potential measurements

ToF-LEIS & ToF-MEIS angular scans measurements (pristine and damaged samples).

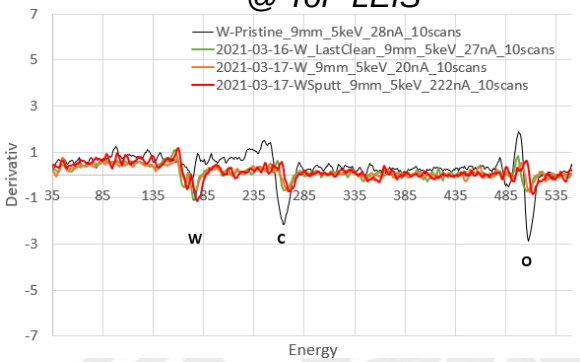
Working-packages

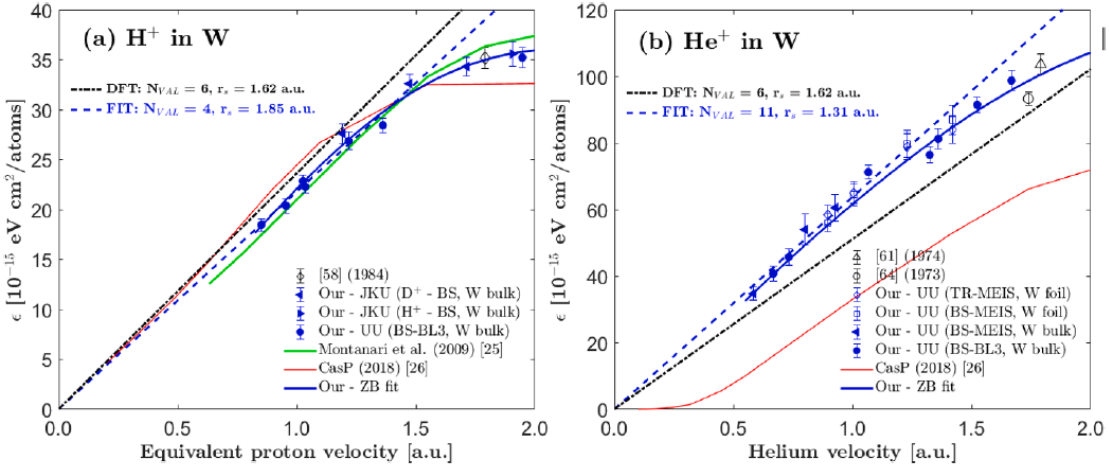
@ UU (VR)

- ✓ Experimental electronic stopping power of Fe, W and EUROFER
- ✓ Experimental interatomic potentials (screening corrections - ToF-LEIS)
- ✓ Assembling QCM @ SIGMA, ToF-MEIS/LEIS set-ups
- ✓ Material deposition and sputtering *in-situ* and simultaneously with near-surface chemical compositional depth-resolved analysis
- ✓ Batch of polycrystalline Fe and W (ex-situ & *in-situ* chemical analysis)
- ✓ Batch of EUROFER97 (e.g., batch #3 from KHT)
- ✓ Batch of ITER-grade tungsten (from KHT)
- ✓ Crystalline Fe and W

Examples...

In-situ W surface cleaning
Aim: energy range [0.5 - 10 keV]
@ ToF-LEIS





M.V.Moro et al., Nucl. Instrum. Meth B **498** (2021)

HR commitment

General management

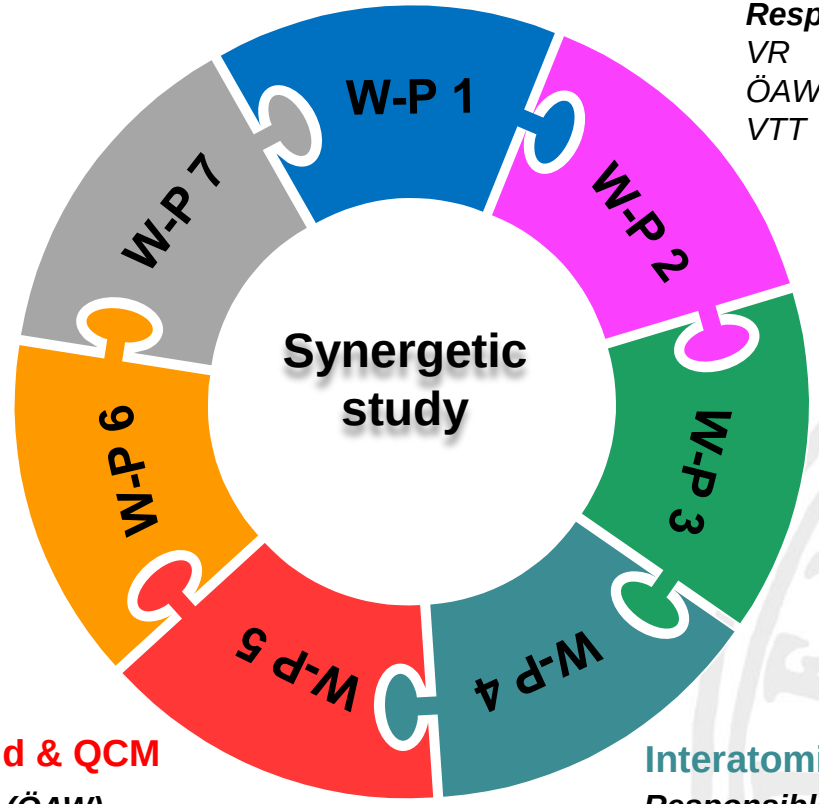
Responsible: MM (VR)
VR → 4.5 pm
ÖAW → 3.0 pm
VTT → 3.0 pm

Computational modeling

Responsible: AS (VTT)
VR → 1.5 pm
ÖAW → 0.0 pm
VTT → 38.0 pm

Sample preparation

Responsible: MM (VR)
VR → 3.5 pm
ÖAW → 1.0 pm
VTT → 1.0 pm



Ion-irradiation experiments

Responsible: MM (VR)
VR → 12.0 pm
ÖAW → 3.0 pm
VTT → 3.0 pm

Electronic energy loss meas.

Responsible: MM (VR)
VR → 7.5 pm
ÖAW → 0.0 pm
VTT → 1.0 pm

Sputtering yield & QCM

Responsible: PS (ÖAW)
VR → 3.0 pm
ÖAW → 35.0 pm
VTT → 1.0 pm

Interatomic potential measurements

Responsible: MM (VR)
VR → 4.5 pm
ÖAW → 4.0 pm
VTT → 1.0 pm

HR commitment

→ Adjustable ←

VR	Participation [pm]			
Researcher	*2021*	*2022*	*2023*	*Total*
MM (PI)	6	6.5	6	18.5
J S-L	2	2	2	6
PS	2	2	2	6
PP	2	2	2	6
Total	**12**	**12.5**	**12**	**36.5**

ÖAW	Participation [pm]			
Researcher	*2021*	*2022*	*2023*	*Total*
PS	9	7	3	19
CC	7.5	8.5	11	27
Total	**16.5**	**15.5**	**14**	**46**

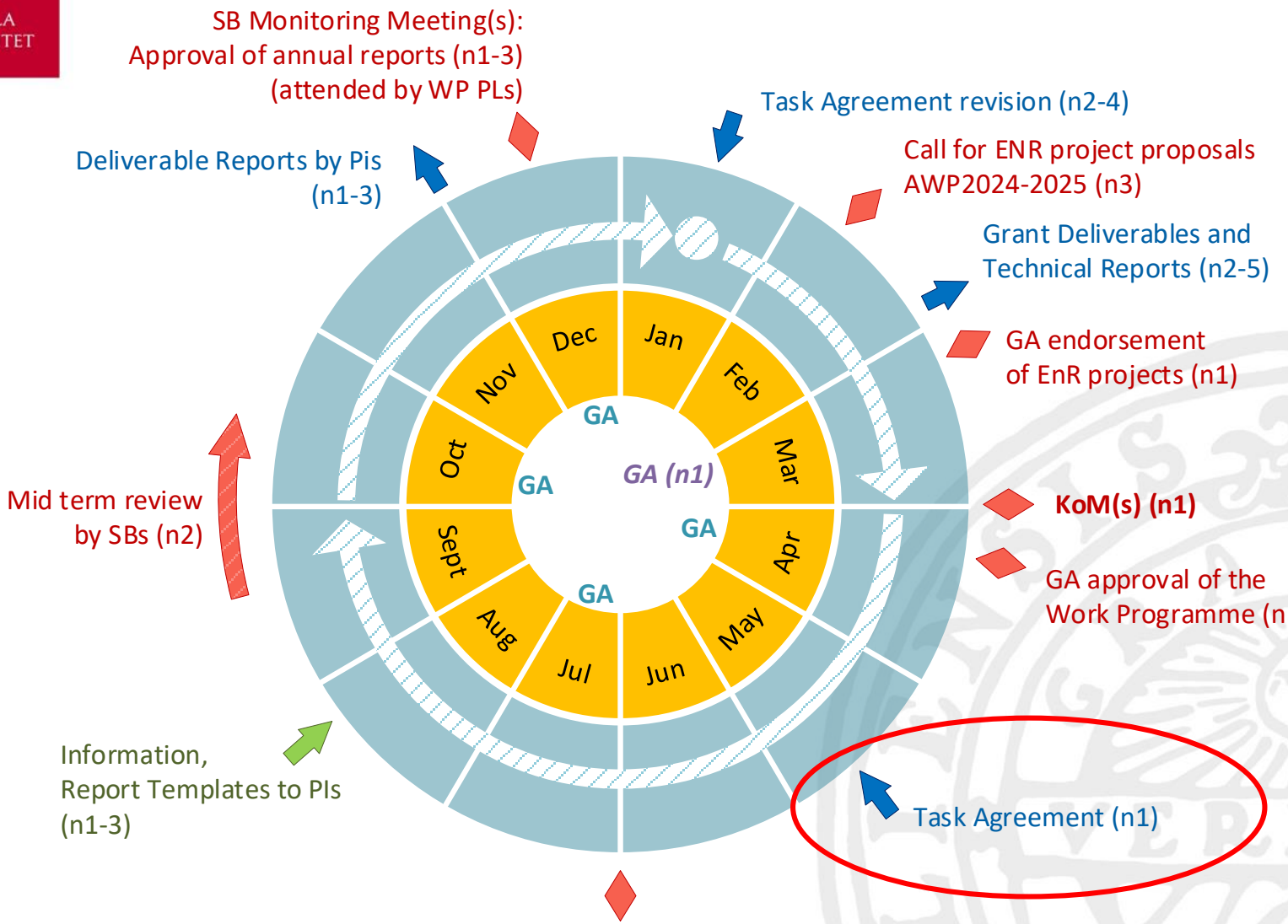
VTT	Participation [pm]			
Researcher	*2021*	*2022*	*2023*	*Total*
AS	6	6	6	18
PhD-student	10	10	10	30
Total	**16**	**16**	**16**	**48**

Personnel, goods & services

Financial data including indirect costs (x1.25)	2021			2022			2023		
	VR	ÖAW	VTT	VR	ÖAW	VTT	VR	ÖAW	VTT
Personnel cost (k€)	98	130	125	102	122	125	98	110	125
Goods & services (k€)	24	5	0	31	5	0	26	5	0
Hardware (k€)	3	0	0	3	0	0	3	0	0
Travel (k€)	4	8	4	4	8	4	4	8	4
Total (k€)	**129**	**143**	**129**	**141**	**135**	**129**	**131**	**123**	**129**

Total over 3 years (k€)	1188
50% of total (k€)	**594**
Consortium contribution (k€)	**588**

ENR - life cycle



Modified from D. Kalupin - 2021-03-18

Communication

- **IMS – information (financial) management**

Contractual information. Also to be used to manage all the **missions (travels, etc)** by the participants. https://IMS.euro-fusion.org

- **IDM – document management**

Contractual documents (e.g. Task Agreement) and uploading reports. **PI** will be granted access. https://IDM.euro-fusion.org.

- **WIKI pages – project documenting area**

Wiki page accessible to all EUROfusion members. **Document**: team, deliverables, scope, meetings, results, WPs links, use of experimental data, reports, publications. https://wiki.euro-fusion.org/wiki/Project_No5

- **INDICO – meetings & presentations**

Organise **meetings & store materials**. Materials uploaded there will remain for the entire Horizon Europe framework (at least). https://indico.euro-fusion.org/category/305/

Publications

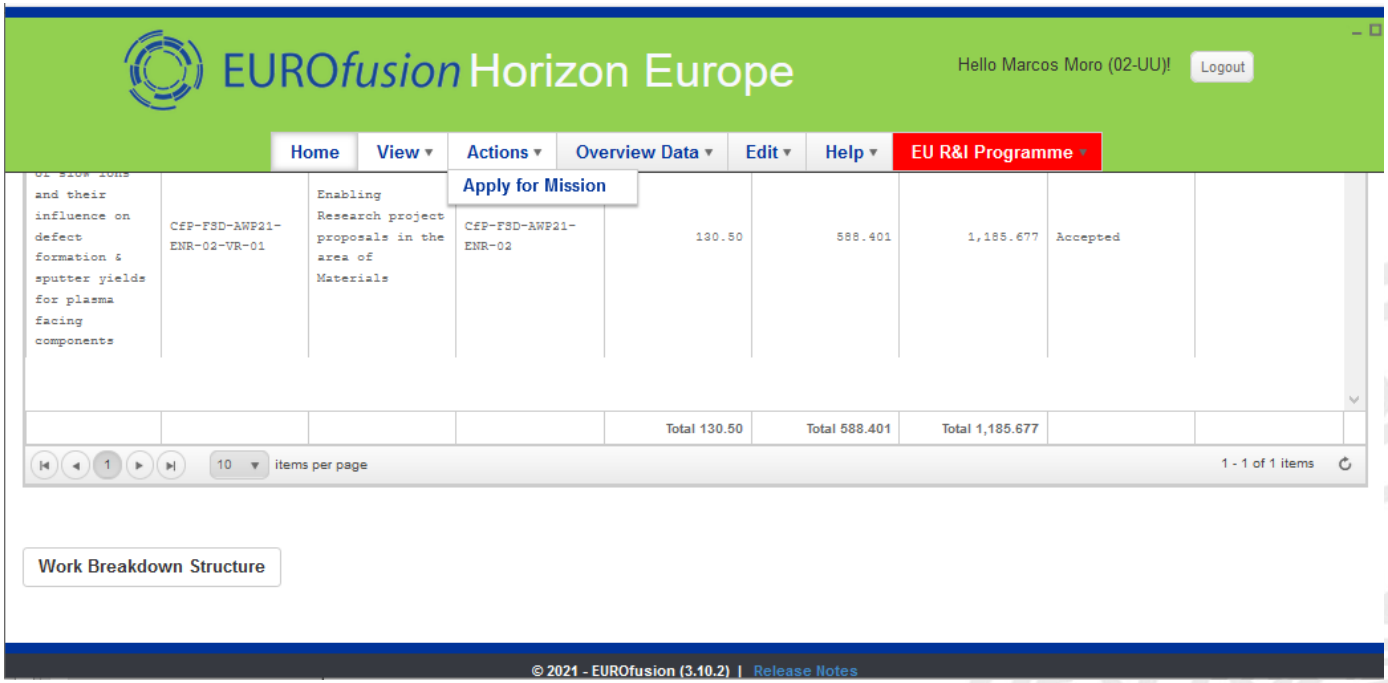
- ENR-related publications (and presentations, etc) to international conferences must be submitted for approval at the **EUROfusion pin board**: https://users.euro-fusion.org/webapps/pinboard/EFDA-JET/.

- **The approval** of publications must also be done **by the PI.**

- These publications should have **the EUROfusion disclaimer** in the acknowledgement and the final author manuscript version of the paper (before it is typeset by the publisher) needs to be provided for the EUROfusion repository.

Missions

IMS



1. No *Unit Costs*, all missions will be done on *Actual Costs*
2. Tickets are eligible;
3. Support level up to 70% (indirect costs are eligible)
4. Application needs approval by PI

Missions

- Discussions...
- Official starting date
- Fine-tunes - (if yes, please feedback within ca. 1 week)
- etc...

Discussed points

Major after meeting outcomes:

1. Participants:
   - VR: MM, PS, J S-L, PP, DP
   - ÖAW: PS, CC, FA
   - VTT: AS
   - PMU: DK

2. Agreed project time-frame:
   - Starting date: May 1st 2021.
   - Ending date: May 2024 (3 calendar years).

3. Keep *tasks & deliverables* regarding 2022 and 2023 calendar years as they are.

4. Shift (few months) the tasks & deliverables from W-P 7 due to recruitment of a new PhD-student (Aalto University - AS). Recruitment process ongoing.

5. Based on (3) and (4): mounting the final task-chronogram after final feedback from VR-ÖAW-VTT.

6. Regular ENR meetings to happen once a month (scheduled by PI via INDICO).