



The European Materials Modelling Council

VIRTEX-MECM

1. Call/topic number DT-NMBP-10-2019: Translation of manufacturing problems into materials modelling, ***possibly in combination with*** DT-NMBP-09-2018: Accelerating the uptake of materials modelling software
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3. Name/subject **VIR**Tual **EX**ploration of Molecular Energy **Conversion** Materials (**VIRTEX-MECM**)

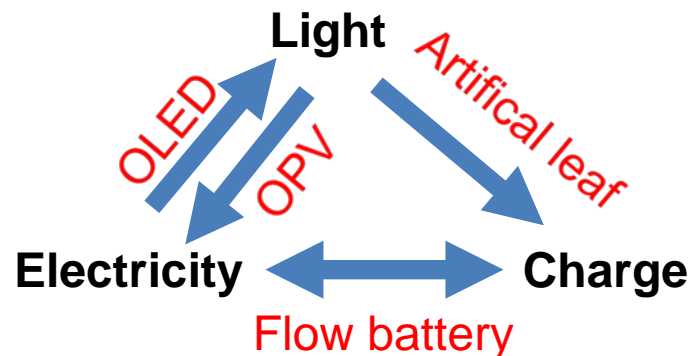


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Objectives VIRTEX-MECM

4. Objectives

- Provide **(European) manufacturing industry** with integrated set of modelling tools for virtual exploration of MECMs to optimize fabrication processes (**OLED**, **OPV**, **Flow battery**, **Artificial leaf**, ...)
- Strengthen ecosystem of **European software companies** selling software for modelling of (devices of) MECMs
- Build coherent **European academic community** performing world-class modelling research of (devices of) MECMs and focusing on long-lasting valorization





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Innovative and expected results VIRTEX-MECM

5. Innovative aspects

- **fully predictive** (based on *ab initio* calculations)
- **fully multiscale** (from molecule to device)
- **fully integrated** (seamless connection of tools)
- **fully virtual** (every aspect is modelled)

6. Expected results

- Bring (existing) modelling tools from TRL 4 to TRL 6
 - Develop links between modelling tools at TRL 6
- **Integrated set of modeling tools at TRL 6**



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Expected results and demo VIRTEX-MECM

7. Expected impact

- Better performing products, optimized production processes, reduced production costs, higher profit margins of the **(European) manufacturing industry** producing (devices of) MECMs
- Flourishing (profits, jobs) **European software companies** selling modelling tools for (devices of) MECMs
- Excellent **European academic community** focusing on valorization

8. Demo

- Demonstration of successful resolution of a **specific manufacturing problem** by virtual exploration of MECMs



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Possible partners VIRTEX-MECM

9. Possible partners (tentative and definitely not exclusive !)

Manufacturing:



Software:



Academic:

