Current trends in the functional oxides development

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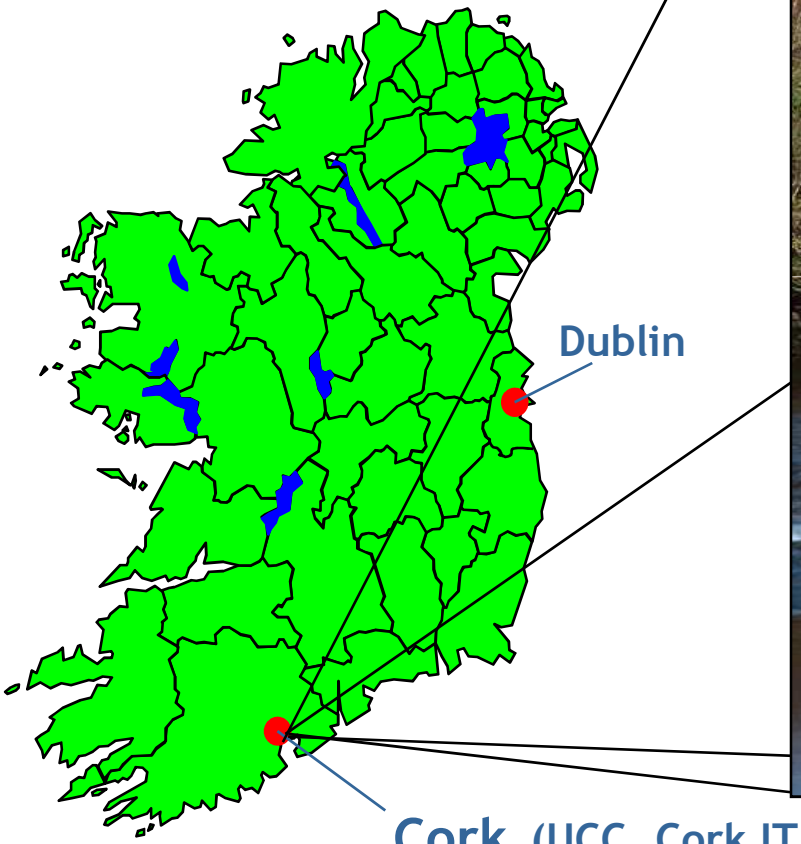
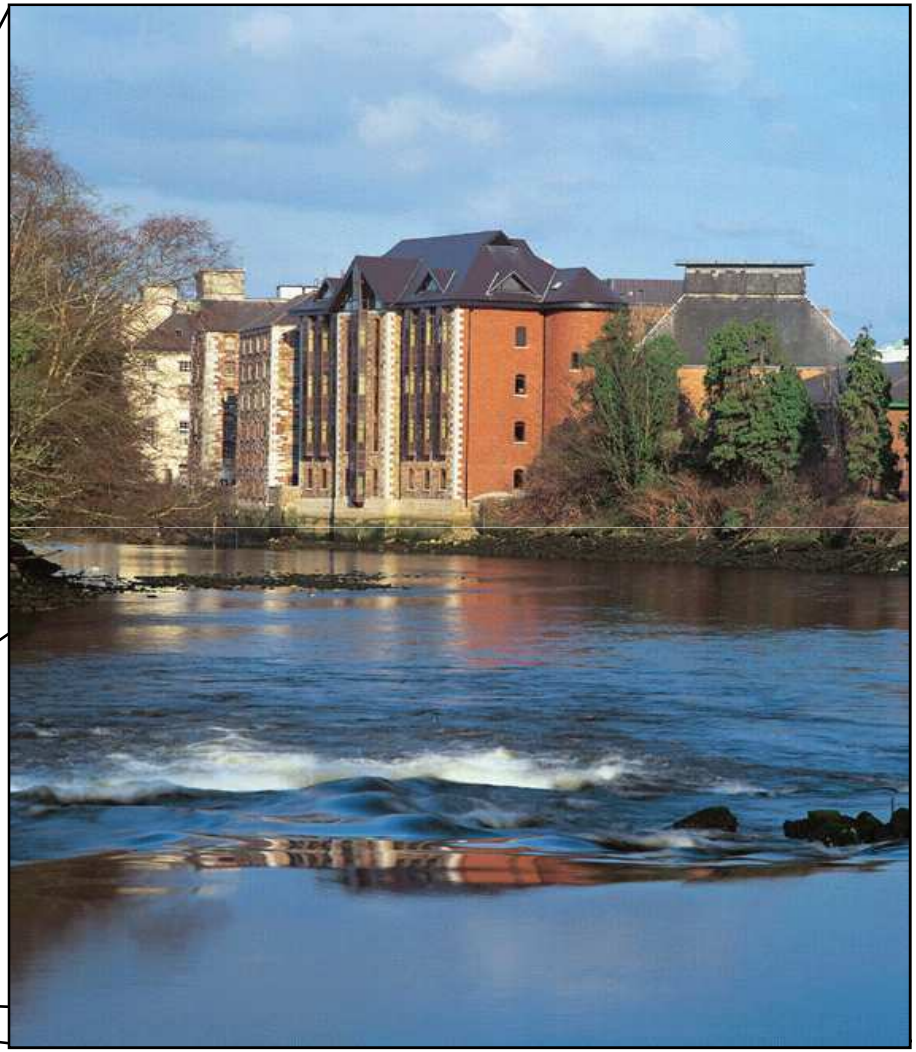
Tyndall National Institute

- Based in Cork, at Lee Maltings





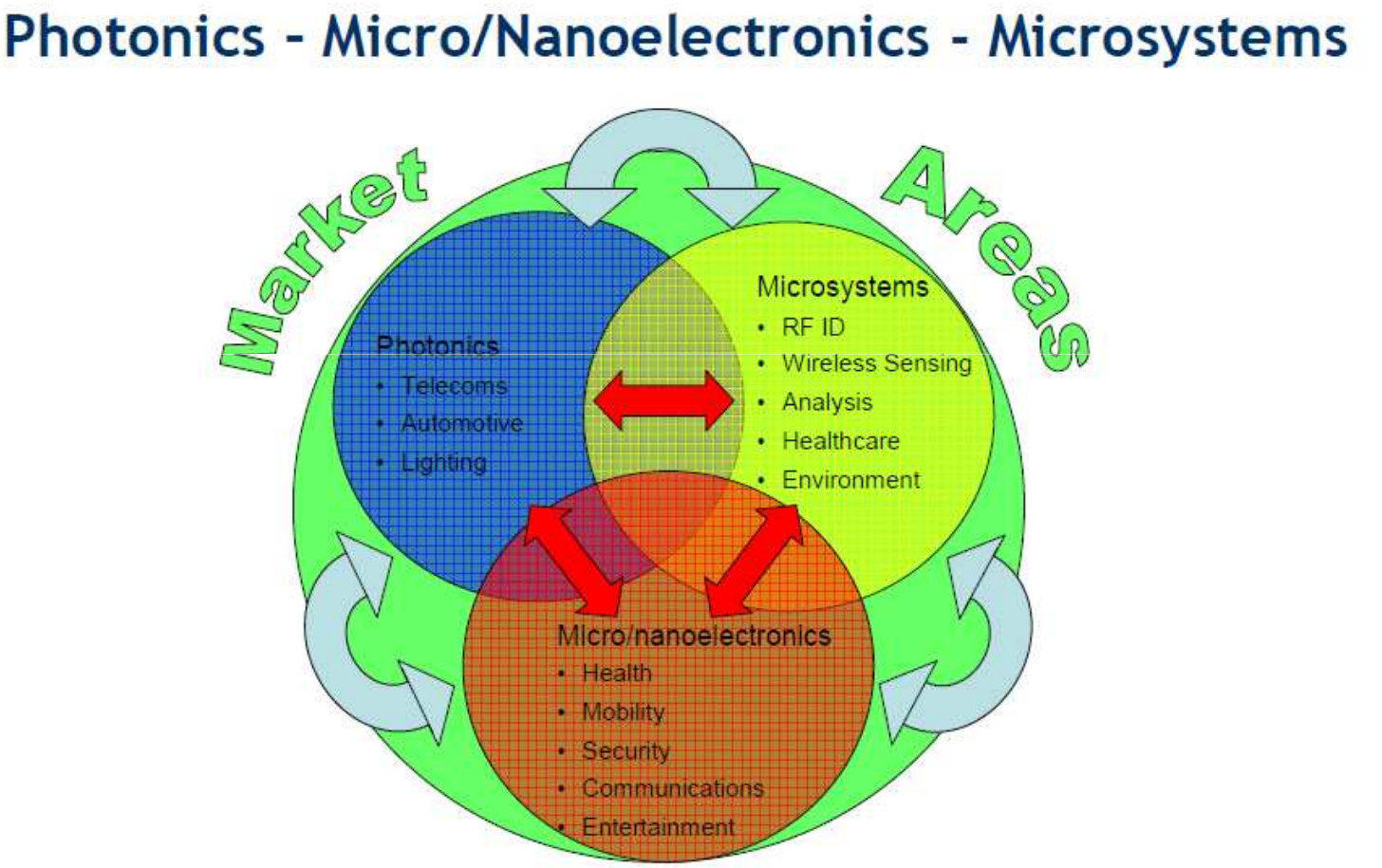
Tyndall National Institute

- Established in 2004
- Brings together researchers in:
  - Photonics
  - Micro/Nanoelectronics
  - Nanotechnology
  - Microsystems
  - Life Sciences
- Originally from the National Microelectronics Research Centre (NMRC), University College Cork (UCC) and Cork Institute of Technology (CIT)
- >450 research engineers, scientists, students, interns & support staff

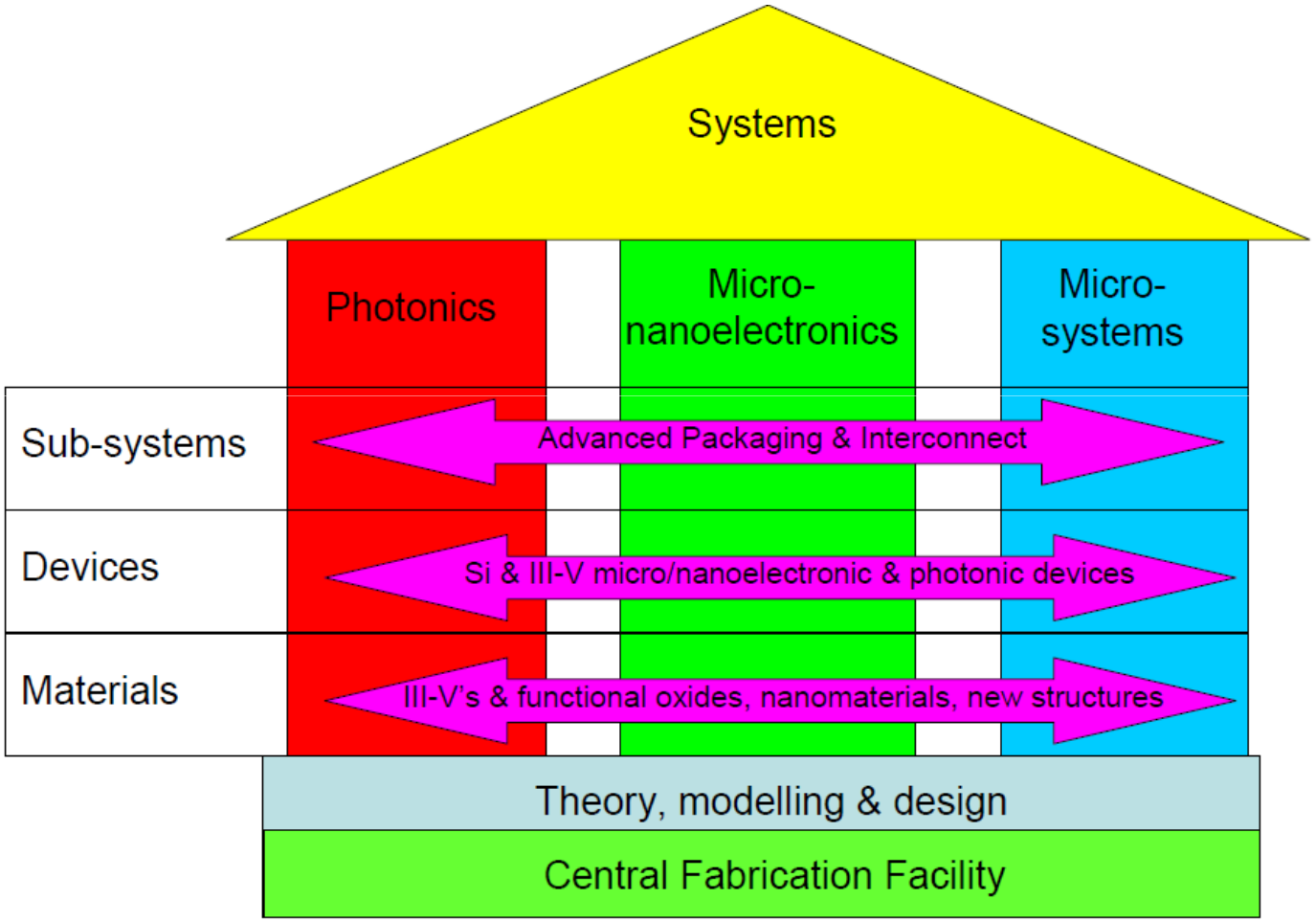
Mission Statement:

“Tyndall will be a Centre of Excellence for research, development and graduate training in Information and Communications Technology, recognised internationally for the quality of its outputs in materials, devices, systems and people, and its creation of new opportunities for Ireland’s economic growth .”

Tyndall's Activity Areas



Tyndall research concept: “from atoms to the systems”



Why material development are technological relevant? *See for example FP7 NMP program*

“Better mastering of materials has characterised the development of human societies since the dawn of humanity.

At the present time, 70% of all technical innovations depend directly or indirectly on the properties of the materials and their use, and this percentage is expected to increase further.

Therefore, at European level, materials have been identified as one of the Key Enabling Technologies for Europe”

Why functional oxides?

Because of their many technological applications…

Moisture Barriers

Photocurrent Blocking Layers

Photocatalytic Materials and Coatings

Interface Control Layers

UV Detectors

Anti Microbial Films

Surface Functionalisation

Pore Size Control Filtration

Flame Retardant Coatings

Enhanced Electrical and Thermal Conductivity

+ Many More

Current trends on material development

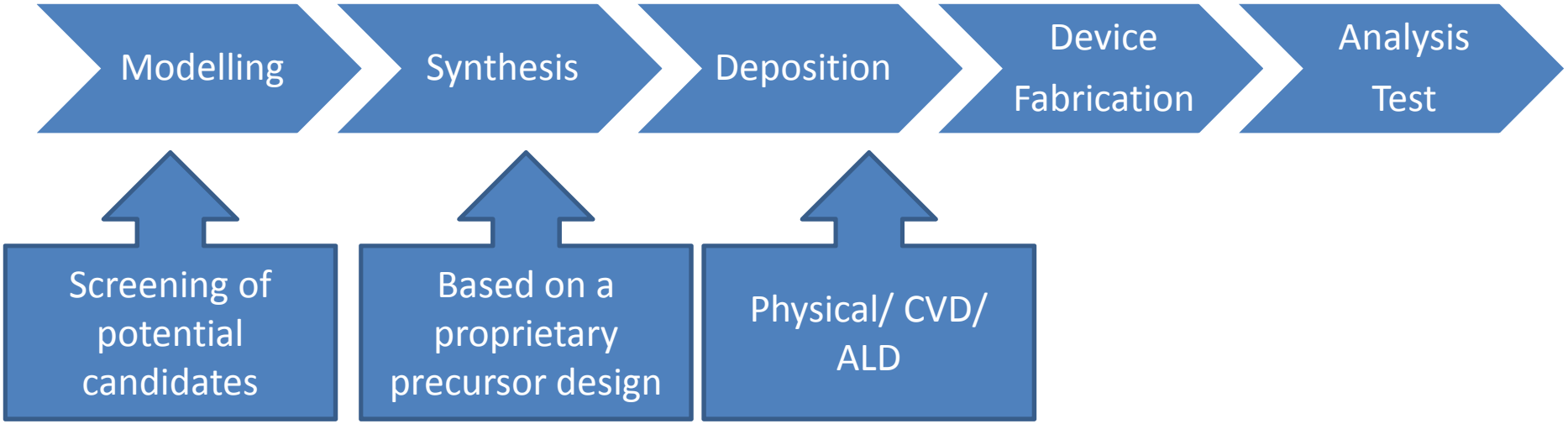
- Lucky/accidental discovery: hardly this approach can significantly boost technical innovation

- Material design based on some analogy with some other existing materials: serial approach as research methodology (one by one approach, slow, time consuming and costly)

- High-throughput combinatorial approach: parallel approach where for example one material properties is changed (e.g. the concentration of a dopant); a library of samples with various composition is generated in a single run and then analysed (using sometime robotic systems) in order to identified the best composition. When employing robotic system up to 40-100x increase in samples analysis throughput. Requires a heavy investment

- Material discovery based by a rational design; Allow a fast screening of potential candidates who will fulfil the end-user requirements. With the fast approaching of pentaflop computing era this may represent the most fruitful way forward

Tyndall research concept for material development based on a rational design



FP6 STREP NATCO methodology for new TCOs

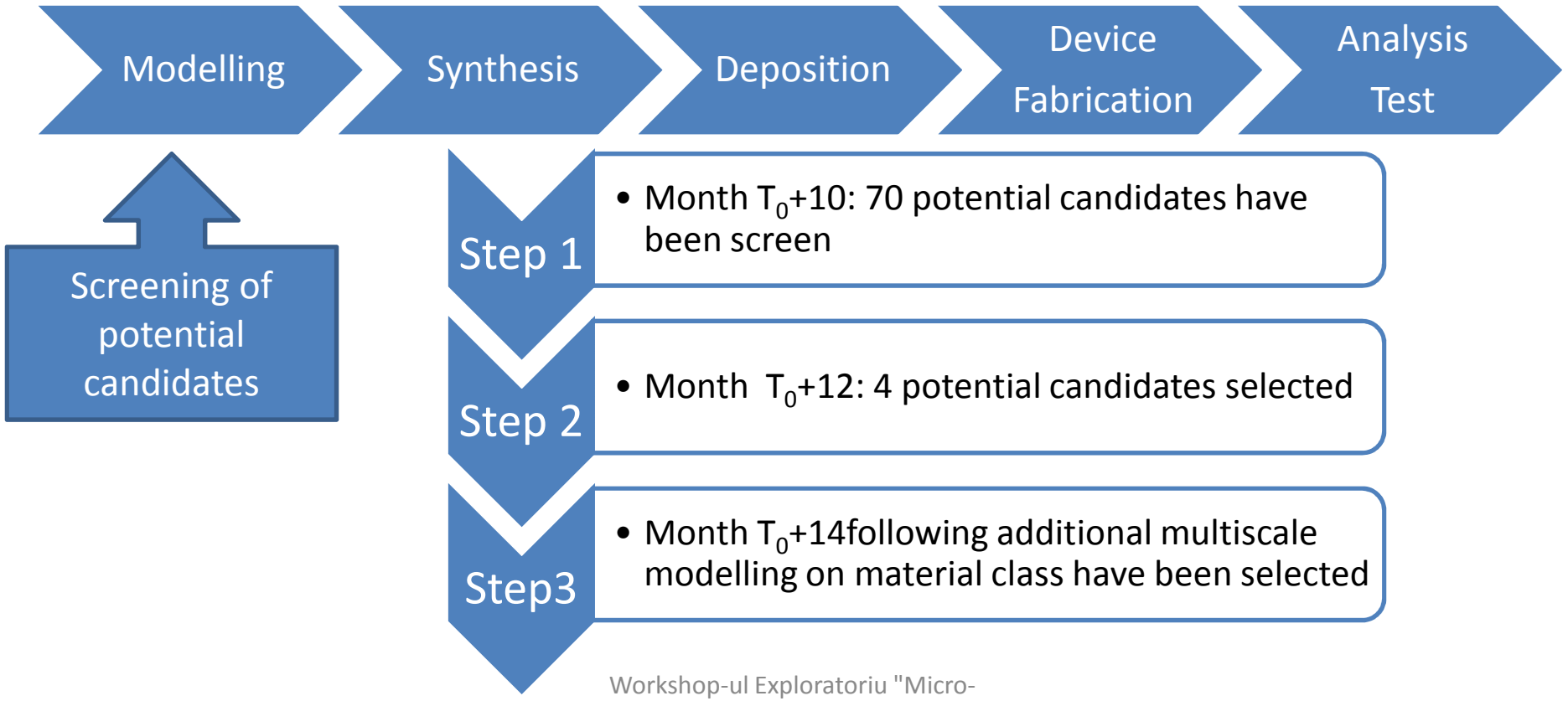
-Choice of prototype material: NATCO choice was Cu_2O

-First principles modeling is used for a better understanding of the mechanism behind the p-type TCO properties of the prototype material

-First principles studies of doping and alloying Cu_2O prototype to propose new p-type TCO candidates

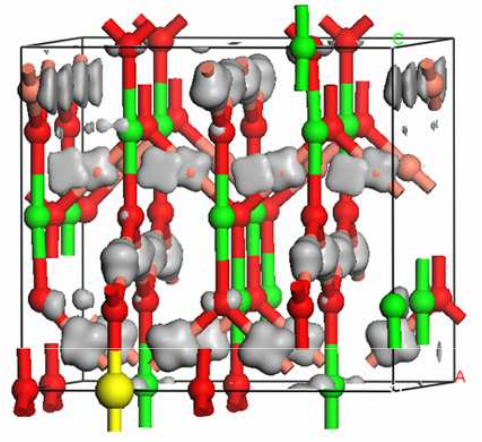
-In depth studies of optical, microstructural and electrical properties of p-type TCO candidates, both as bulk and as thin films

FP 6 NATCO research methodology

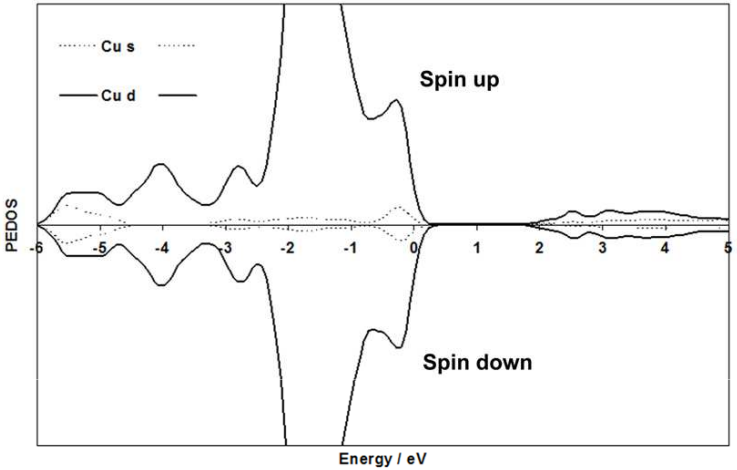


New material selection: Ba^{2+} Doping in $SrCu_2O_2$

Design rule proposed: Dope $SrCu_2O_2$ with cations that have a larger ionic radius than Sr and do not introduce band gap states : predict ***Ba-doped $SrCu_2O_2$ as p-type TCO with larger band gap***



delocalised hole state upon Cu vacancy formation

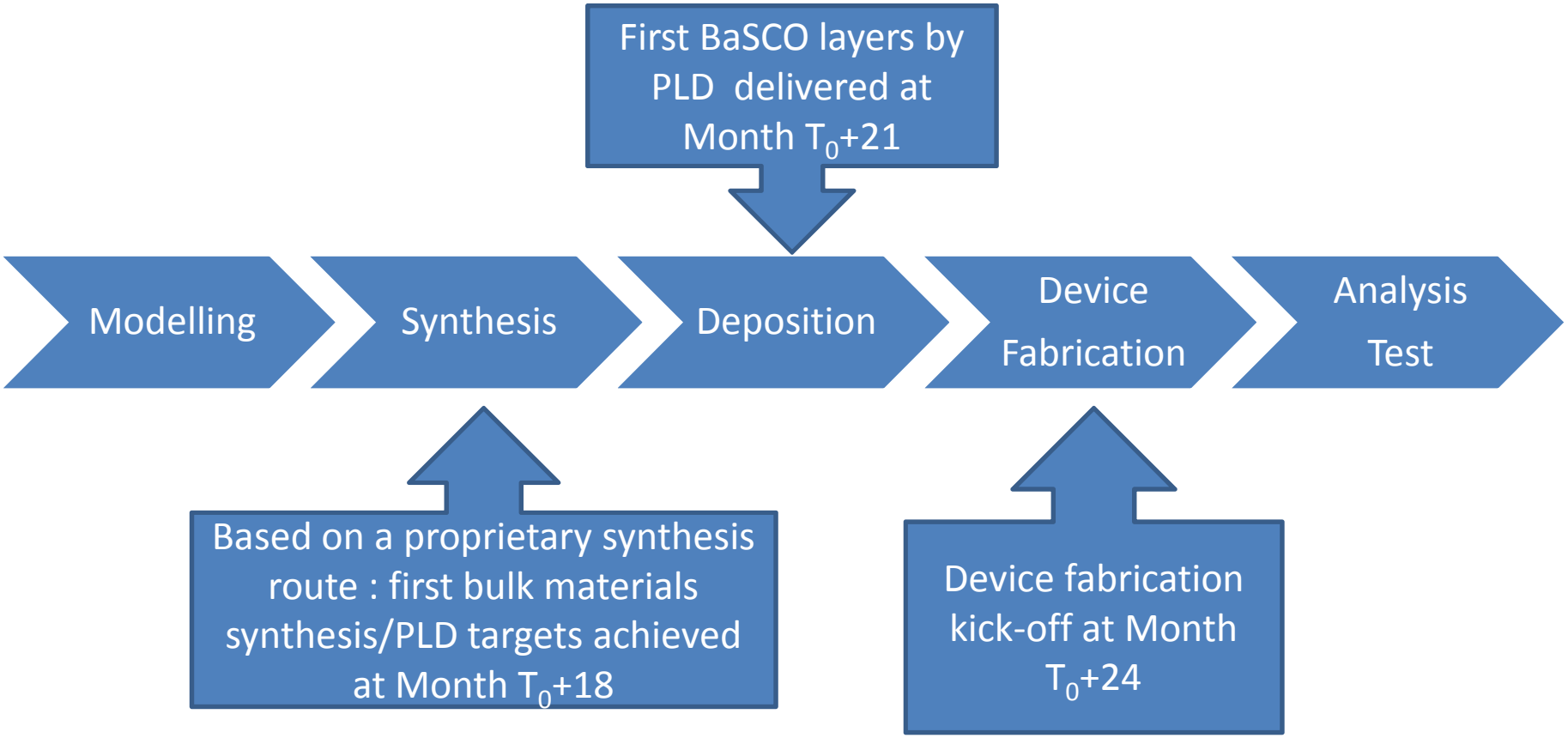


Material	E_g (eV)	m* / m_e
$SrCu_2O_2$	1.82(DFT) 3.20(Hybrid DFT)	-1.48, -0.91, -6.66
6% Ba doped $SrCu_2O_2$	1.97(DFT) 3.24(Hybrid DFT)	-1.68, -0.88, 37.71, -9.43

→ Ba doping: enhanced band gap and reasonable effective masses

EU FP 6 IST FET OPEN project NATCO

FP 6 NATCO research methodology



Conclusion

- Novel materials development represent a “Key Enabling Technologies for Europe”
- Material discovery and development based on a rational design was identified as a potential way forward
- When combining this approach with that of high-throughput combinatorial screening a fast track process will results allowing the timely introduction to market of the novel technologies based on these materials