2DFUN

www.2Dfun.eu

# 2DFUN - 2D FUNCTIONAL $MX_2$/GRAPHENE HETERO-STRUCTURES

FLAG-ERA JTC 2015 PROJECT KICK-OFF APRIL 13, 2016, BUDAPEST, HUNGARY

MATTY CAYMAX, PROJECT COORDINATOR

imec

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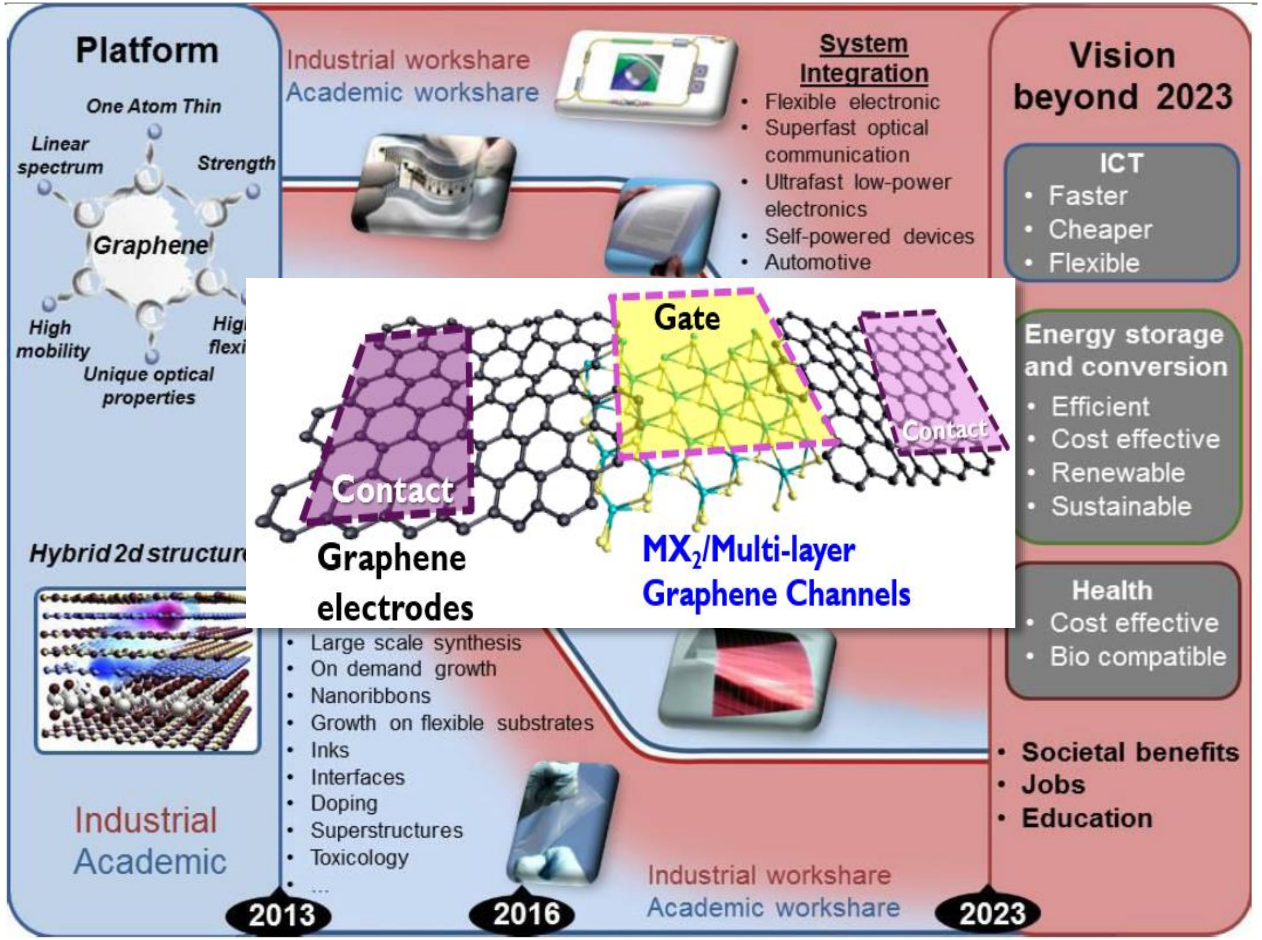
# 2D MATERIALS – GRAPHENE AND BEYOND

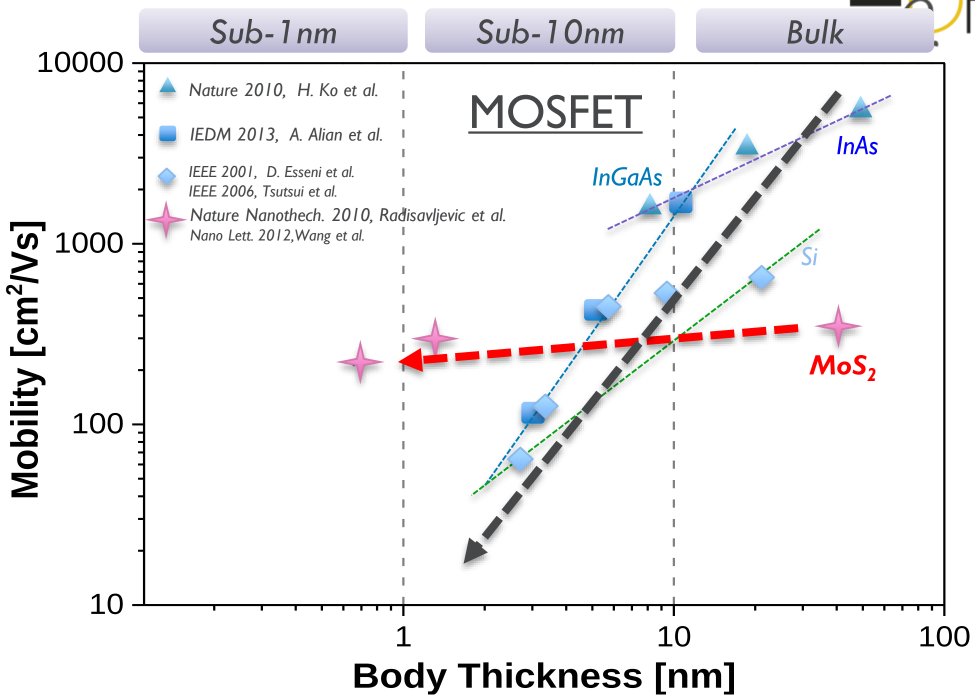
## VISION AND TIMELINE

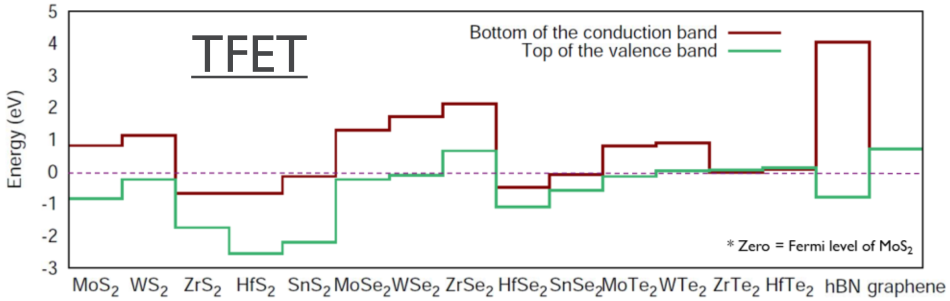



Jari Kinaret, “Graphene Flagship” presentation “ Working together to combine scientific excellence and technological impacts”, 2012

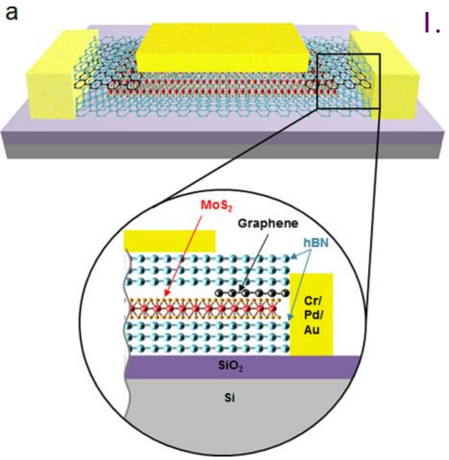
# WHY $MX_2$ FOR TRANSISTOR SCALING?

- $MX_2$: interesting properties for ultra-thin body devices
  - 2D crystals with VdW bonding – no lattice mismatch issues
  - High DOS
  - Reasonable mobility, especially for ultra-thin channels
  - Low dielectric constant helps reducing short-channel effects (planar devices)
  - Wide band gap and wide choice of BGs allow BG engineering in TFET
  - Low density of dangling bonds on surface reduce defect density



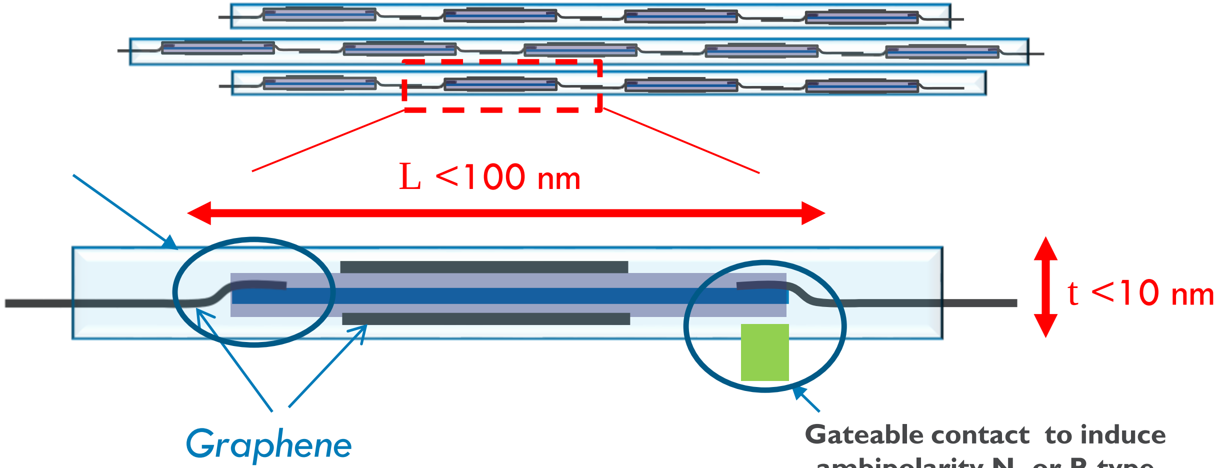



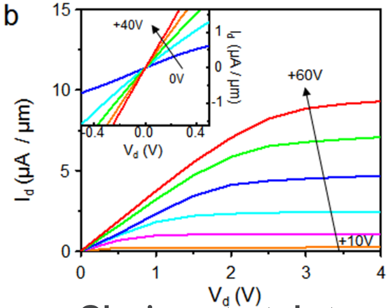
# WHY GRAPHENE/$MX_2$ HETERO-STRUCTURES?



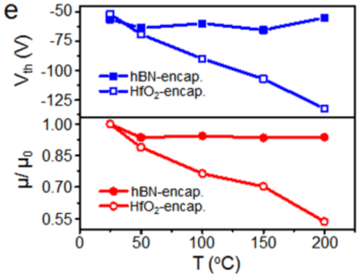

Lee et al. ACS Nano DOI: 10.1021/acsnano.5b01341

1. Contacts to $MX_2$ are bottleneck
   - Graphene/$MX_2$ ohmic contacts shown
   - Challenge is long-term stability




Ohmic contacts between MoS2 and Graphene



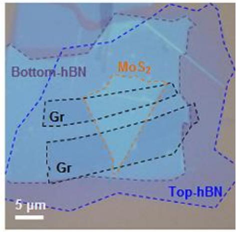

Challenge : long term stability

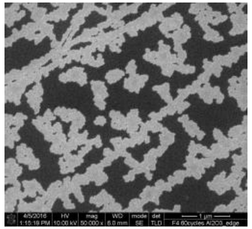
2. Circuit scaling approach:
   - Electrolytic gating of a $MoS_2$ flake shows ambipolar conduction
   - $MoS_2$ is normally n-type
   - **Smaller XOR** can be built with 2 gate transistors
   - 4 devices rather than 8 needed for same logic operation
   - Possible because of the *ability to reconfigure* the devices
   - 3D scaling through stacking of devices possible

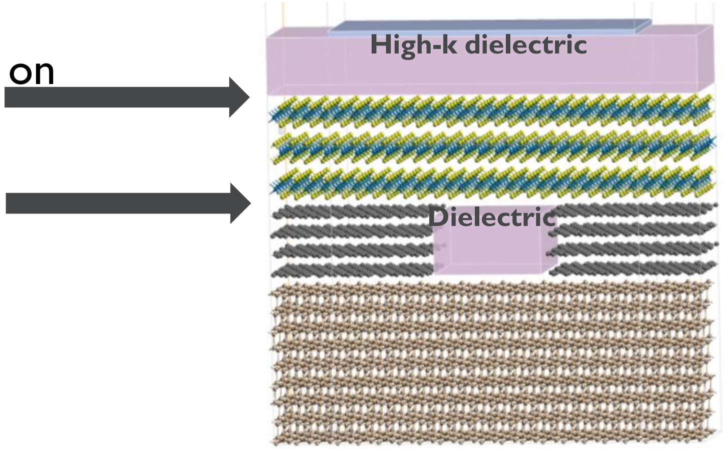
# CHALLENGES

## $MX_2$ MAKING AND DEVICE STRUCTURE

- Synthesis of high-quality 2D $MX_2$ layers with controlled thickness on large wafer size (300mm)
  - No reliable processes known/developed
  - No commercial reactors available
- Growth of layers on saturated, passive 2D surfaces (graphene, $MX_2$)
  - Requires surface functionalization
- Importance of interfaces:
  - Interface between $MoS_2$ and Gate dielectric: Effect on mobility, hysteresis, reliability
  - Contact between $MoS_2$ and graphene:
    - Ohmic? Contact resistance?
    - Coping with high current densities?
    - Scaling potential?



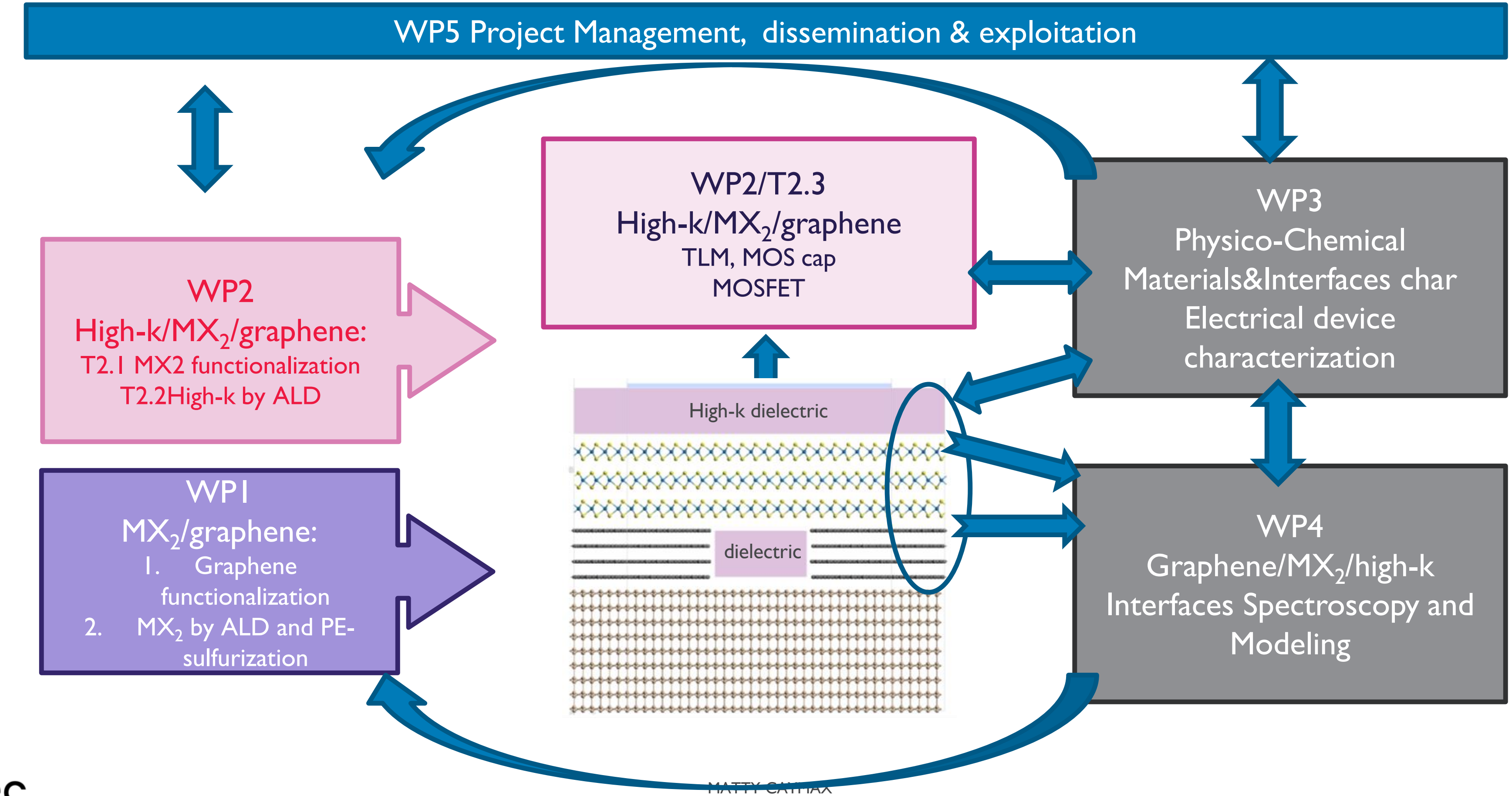





# 2DFUN OBJECTIVES

- Technological Objectives
  1. Develop large-area deposition process for $MX_2$ on graphene
     1. Low-T sulfidation (plasma enhanced) of ALD-grown metal or metal oxide layers
     2. Direct growth from gas phase (ALD, CVD) with M and X gas-phase precursors
  2. Develop high-k dielectric growth process on $MX_2$
  - Surface functionalization of graphene and $MX_2$ for these growth processes
- Scientific Objective:
  1. Obtain fundamental insight in chemical structure and energy states spectrum at the high-k/$MX_2$ and $MX_2$/graphene interfaces

# 2DFUN PROJECT AND PROJECT LAY-OUT



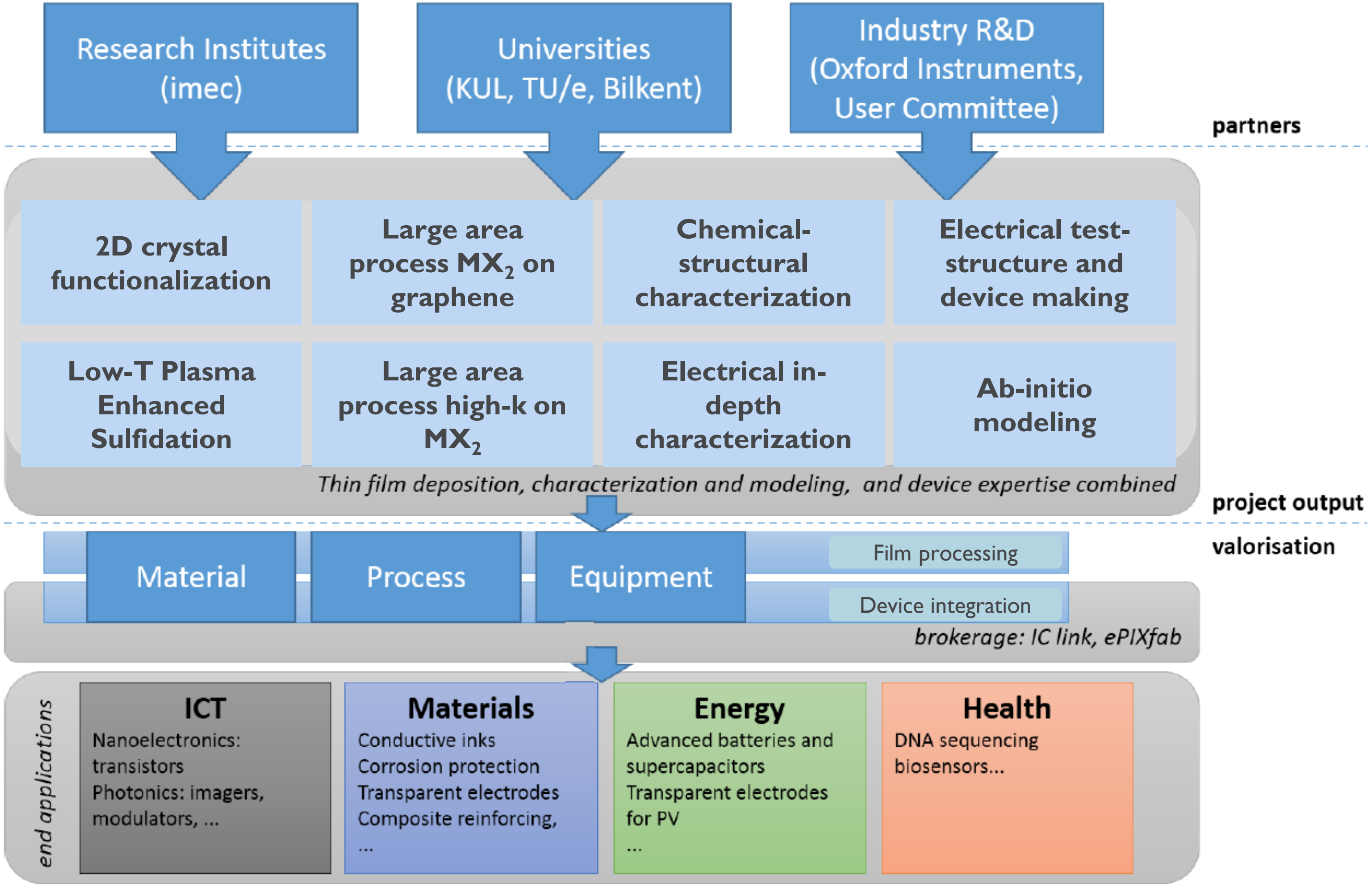
# 2DFUN CONSORTIUM

| | IMEC | KULeuven | TU/e | Bilkent Univ | OI | Total |
|---|---|---|---|---|---|---|
| Type | R&D institute | University | University | University | Company | |
| Location | Leuven, Belgium | Leuven, Belgium | Eindhoven, The Netherlands | Ankara, Turkey | Cambridge, UK | |
| Role | Coordinator | partner | partner | partner | partner | |
| Involvement | WP1, WP2, WP3, WP5 | WP2, WP3, WP4 | WP1, WP3 | WP4 | WP1, WP5 | |
| Budget (euro) | 384909 | 179359 | 249810 | 129000 | 0 | 943078 |

# PARTNERS' TASKS IN 2DFUN

| | IMEC | KULeuven | TU/e | Bilkent University | OI, UK |
|---|---|---|---|---|---|
| Growth | $MX_2$ on graphene<br>High-k on $MX_2$ | | $MX_2$ on graphene | | Reactor hardware for TU/e |
| Surface functionalization | | Graphene and $MX_2$ functionalization | | | |
| Electrical test structures | MOS caps, TLM, MOSFET | | | | |
| Interface, film and electrical characterization | General physical, chemical and electrical | In-depth interface characterization (ESR, IPE) and electrical measurements | General physical and chemical | In-depth (e-XPS) | |
| Fundamental structural modeling | | Atomistic interface and defect modeling | | | |

# IMPACT




- NRFO in Belgium: VLAIO
- Strong industrial link via industrial partners:
  - ASM Belgium
  - AMAT Belgium
  - LAM Belgium

# $MX_2$ LAYER SPECIFICATIONS TO BE REACHED

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| Requirements | Target | Measurement technique |
|---|---|---|
| Uniformity | 100- 300mm Si wafer scale | Spectroscopic ellipsometry |
| Number of layers | Controlled between 1-5 | Raman, RBS; For a single layer: M content= 1.2E+15 at/cm$^2$ |
| Composition | W/S = ½ | Rutherford Backscattering Spectroscopy |
| Impurity content | < 1 at% | Elastic Recoil Detection, XPS |
| Crystallinity | Monocrystalline, basal plane parallel to the substrate surface<br>Domain size > 50µm$^2$ | GI-X-Ray Diffraction, Transmission Electron Microscopy, Atomic Force Microscopy, Photoluminescence mapping |
| Layer continuity | Normalized substrate intensity < 1% | TOFSIMS |
| Contact resistance | < 400 ohm.µm | I/V measurement on TLM |
| Mobility | 20 cm$^2$/Vs | Split CV in MOSFETs |

# EXPLOITABLE RESULTS

## TARGETED INDUSTRIALLY VIABLE PROJECT OUTCOMES

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| Exploitable result | TRL at project start | TRL target | Comment |
|---|---|---|---|
| **Process for manufacturable sulphurization of transition metal layer** | 3 | 5 | Advancing from known post-process sulphurization of coupons to in situ (no vacuum break) sulphurization of 300mm wafers |
| **Process for growth of $MX_2$ layer on an 'inert' layer such as graphene** | 2 | 3 | Advancing from no prior demonstration to success on (coupons distributed over) a 300mm wafer |
| **Process for growth of high-k dielectric on $MX_2$ layer** | 2 | 4 | Advancing from no prior demonstration to results on 200 and/or 300mm wafers |
| **Manufacturing process flow for a functional $MX_2$-based MOSFET** | 2 | 4 | Advancing from results based on exfoliated layers to a lab-flow on coupons |
| **Process tool specifications capable of delivering the project process advances** | 3 | 4 | The project has only minor hardware developments, but will validate the necessary features of process tools required to exploit these methods |

# DISSEMINATION OF RESULTS AND TRAINING ACTIVITIES

- Website hosted by imec: www.2Dfun.eu
  - Public domain information only
  - Project description, consortium, members,...
  - Annual reports
  - Public deliverable reports
  - Partner publications, presentations...
  - Useful links
- Presence on other websites
  - FLAG-ERA website
  - Graphene Onboard Website of Graphene Flagship
  - Imec's internal project website = restricted area for IWT SBO participants
- Workshop(s)
  - To be organized at/by imec as satellite event of imec PTW (April or October)
- Publications & Conference presentations
  - all partners
  - Papers & presentations posted on website

# INTERACTION WITH GRAPHENE FLAGSHIP

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- Complementarities
  - WP3 - Enabling Materials
    - growth on large area substrates
    - in-depth fundamental understanding of the interfaces in 2D hetero-structures
  - WP8 - Photonics and Optoelectronics
    - direct bandgap in single layer $MX_2$, as part of graphene/$MX_2$ hetero-structures
  - WP9 - Flexible electronics
    - low-temperature growth techniques, without the need for transfer
  - WP10 - Wafer-Scale System Integration
    - CMOS compatible graphene processing modules for integration schemes which are scalable to sub 10nm dimensions on industrial wafer scale (300mm)
- Foreseen interactions
  - WP3 to provide various graphene samples to help benchmarking graphene/$MX_2$ and $MX_2$/high-k oxide stacks:
    - Graphene flakes for transfer onto Si substrate?
    - Graphene on Si substrate?
    - Natural or synthesized graphene?
  - WP3 to collaborate in the characterization of 2Dfun $MX_2$/graphene samples
  - WP9 to look into possible use of the graphene/$MX_2$/high k-oxide stacks for opto-electronic applications

# FIRST RESULTS

- WP1&2 - KULeuven chemistry dpt, TU/e and imec: functionalization of graphene, high-growth on 2D materials
  - A suitable molecule for graphene functionalization was identified, and its thermal stability studied.
  - First Al2O3 layer growth on functionalized graphene by thermal ALD shown to result in nicely closed and smooth layers
- WP1 – TU/e: MoS2 growth by thermal sulfidation of ALD-grown MoO3 shown, as first step towards full PE-sulfidation of same MoO3 layers
- WP4 – KULeuven Physics dpt:
  - IPE study of WS2 and MoS2 on SiO2 shows that the valence band tops of both sulfides are very well aligned, hence the "Common anion" rule is valid for $MX_2$ compounds
  - DFT calculations on a 1ML MoS2 film
    - show how the structures of S and Mo vacancies as well as S and Mo antisites in look like
    - Allow to calculate the g-factor of the same defects

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