



JTC-2019

1 April 2020 – 31 March 2023

Epitaxial **T**ransition **M**etal dichalcogenides  
Onto wide bandgap hexagonal **S**emiconductors  
for advanced electronics



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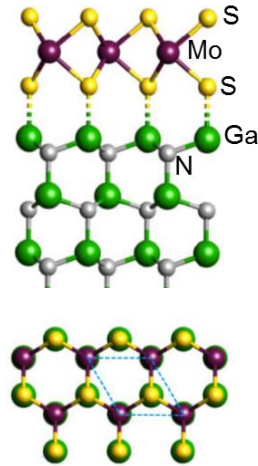
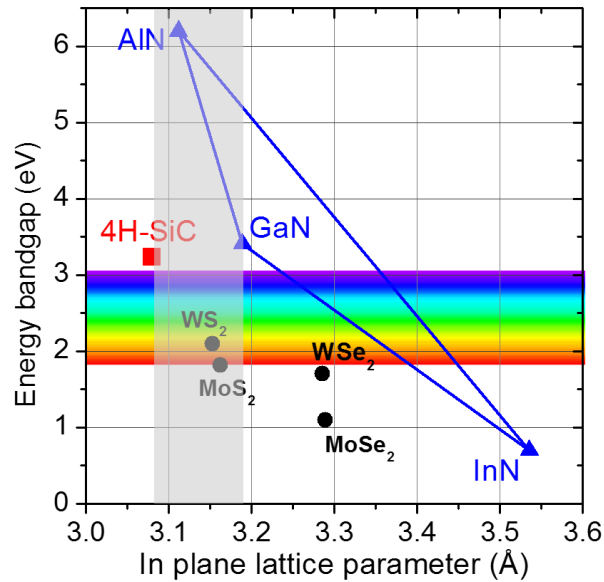
S. Agnello, M. Cannas  
University of Palermo, Italy



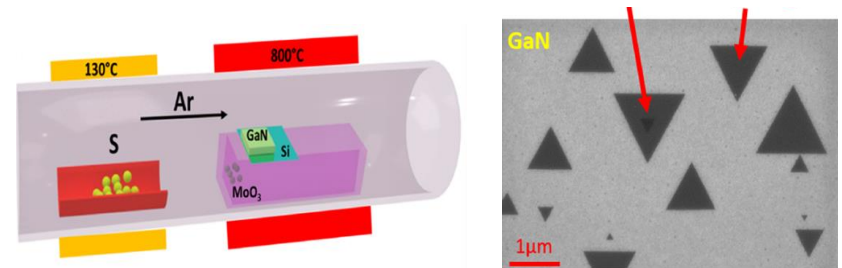
March 16, 2021

# Motivations

- Hexagonal wide band-gap (WBG) semiconductors (4H-SiC, GaN, AlN,  $\text{Al}_x\text{Ga}_{1-x}\text{N}$ ) are nearly ideal substrates for highly oriented epitaxial growth of TMDs

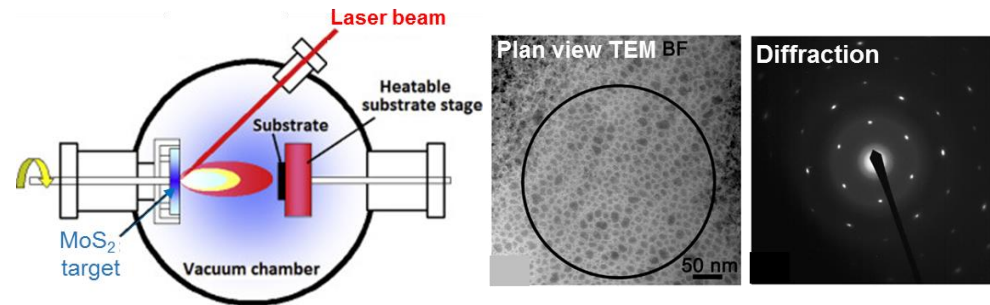


## CVD of $\text{MoS}_2$ on GaN



D. Ruzmetov, et al., ACS Nano 10, 3580–3588 (2016).

## Pulsed Laser Deposition few layer $\text{MoS}_2$ on GaN



S. Chromik, et al., Appl. Surf. Sci. **395**, 232–236 (2017).

- Development of advanced electronic/optoelectronic devices based on the 2D/3D semiconductor heterojunctions between TMDs and WBG.

# ETMOS: Epitaxial Transition Metal dichalcogenides Onto wide bandgap hexagonal Semiconductors for advanced electronics

## Objectives:

- (i) **Epitaxial growth of TMDs** ( $\text{MoS}_2$ ,  $\text{WSe}_2$ ) on WBG hexagonal semiconductors ( $\text{SiC}$ ,  $\text{GaN}$ ,  $\text{AlN}$  and  $\text{AlGaN}$ ) by physical deposition techniques: **molecular beam epitaxy (MBE)** and **pulsed laser deposition (PLD)**.
- (ii) Multi-scale **characterization** (structural, chemical, optical and electrical ) of the grown TMDs; **benchmarking** against materials grown with the same or complementary depositions methods (CVD); **simulations** of the growth process and electronic properties.
- (iii) **Processing** and **device prototypes** based on TMDs/WBG heterojunctions.

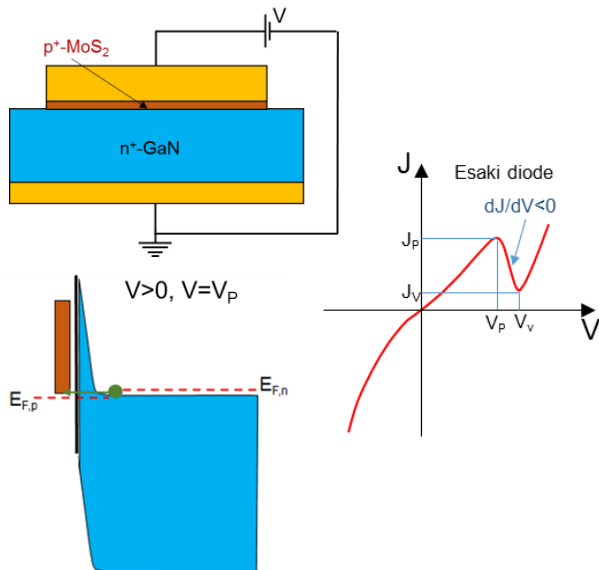
### Low dissipation digital electronics

### Ultra-high frequency (THz) electronics

### Sensors

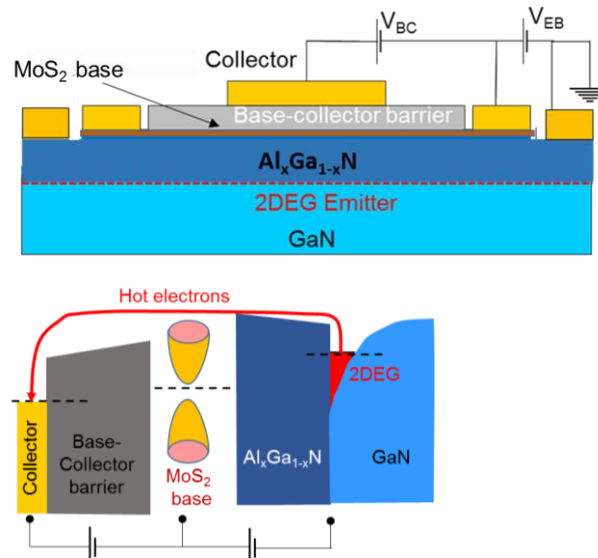
#### Tunnelling diode

$p^+\text{-MoS}_2/n^+\text{-GaN}$  or  $p^+\text{-MoS}_2/n^+\text{-SiC}$



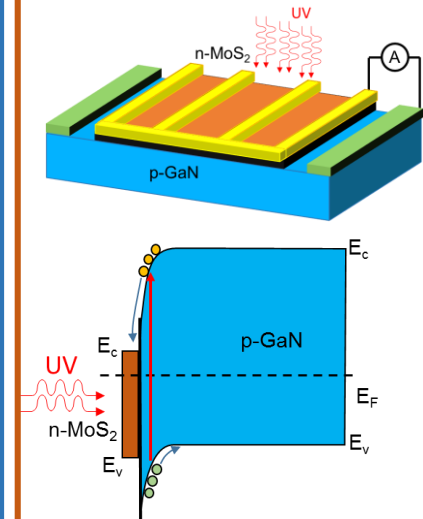
#### Hot electron transistor

$\text{AlGaIn/GaN}$  emitter and  $1\text{L-MoS}_2$  base



#### UV photodetectors

$n\text{-MoS}_2/p\text{-GaN}$  or  $n\text{-MoS}_2/p\text{-SiC}$

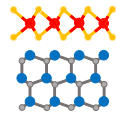




- Nanoscale and device level electrical characterizations.
- Simulations of deposition processes and of electronic transport.
- TMDs/WBG heterojunction devices



- Optical characterizations (Raman, PL) of TMD layers.
- Post growth thermal treatments of TMDs for ex-situ doping
- Electro-optical characterization of TMD/WBG UV photodetectors



## ETMOS Consortium

*5 partners with complementary competences in materials growth, characterization and devices*



- MBE/MOCVD growth of GaN, AlN and AlGaN templates.
- MBE deposition of TMDs ( $\text{MoS}_2$ ,  $\text{WSe}_2$ ).
- Preliminary characterization of substrates and epitaxial layers.

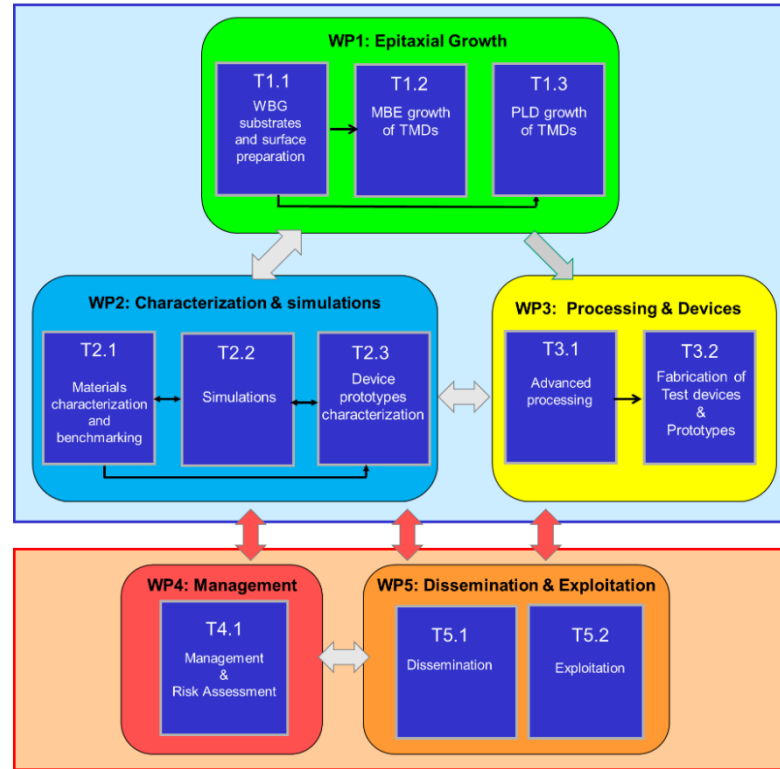


- TEM, STM/STS characterization of TMD/WBG heterostructures.
- CVD growth of  $\text{MoS}_2$  on sapphire and WBG substrates.



- PLD deposition of  $\text{MoS}_2$
- Preliminary characterization of  $\text{MoS}_2$  grown by PLD

# WPs structure



# Gantt

		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36												
		First Year												Second Year												Third Year																							
WP 1 Epitaxial growth	T1.1	[Task]											D1.1	[Task]											[Task]																								
	T1.2	[Task]											[Task]											D1.2	M1	[Task]																							
	T1.3	[Task]											[Task]											D1.3	[Task]																								
WP 2 Characterizations & simulations	T2.1	[Task]											[Task]											D2.1	[Task]																								
	T2.2	[Task]											[Task]											D2.2	[Task]																								
	T2.3	[Task]											[Task]											[Task]											D2.7														
WP 3 Processing & Devices	T3.1	[Task]											[Task]											[Task]											D3.1	[Task]													
	T3.2	[Task]											[Task]											[Task]											D3.2	[Task]													
WP 4 Management	T4.1	[Task]											D4.1	[Task]											D4.2	[Task]											D4.3	[Task]											D4.4
WP 5 Dissemination & Exploitation	T5.1	[Task]											D5.1	[Task]											[Task]											D5.2	[Task]												
	T5.2	[Task]											[Task]											[Task]											[Task]											D5.3			

# Status of activities at M12

1 Apr.  
2020

31 Mar.  
2021

			1	2	3	4	5	6	7	8	9	10	11	12
<b>WP 1</b> Epitaxial growth	<b>Task</b>		<b>Partners</b>											
	<b>T1.1</b>	WBG substrates and surface preparation	<b>CNRS, SAS</b>											
	<b>T1.2</b>	MBE growth of TMDs	<b>CNRS, SAS</b>											
	<b>T1.3</b>	PLD growth of TMDs	<b>SAS, CNRS</b>											
			<b>First Year</b>											
<b>WP2</b> Characterizations & simulations	<b>T2.1</b>	Materials characterization and benchmarking	<b>HAS, CNR, CNRS, SAS, U-Pa</b>											
	<b>T2.2</b>	Simulations	<b>CNR, CNRS, SAS, HAS, U-Pa</b>											
	<b>T2.3</b>	Device prototypes characterization	<b>CNR, U-Pa</b>											
<b>WP3</b> Processing & Devices	<b>T3.1</b>	Advanced processing	<b>CNR, CNRS, HAS, U-Pa</b>											
	<b>T3.2</b>	Fabrication of test devices and prototypes	<b>CNR, CNRS, HAS</b>											
<b>WP4 Management</b>	<b>T4.1</b>	Management & Risk Assessment	<b>CNR, CNRS, SAS, HAS, U-Pa</b>											
<b>WP5</b> Dissemination & Exploitation	<b>T5.1</b>	Dissemination	<b>U-Pa, CNR, CNRS, SAS, HAS</b>											
	<b>T5.2</b>	Exploitation	<b>CNRS, CNR, SAS, HAS, U-Pa</b>											

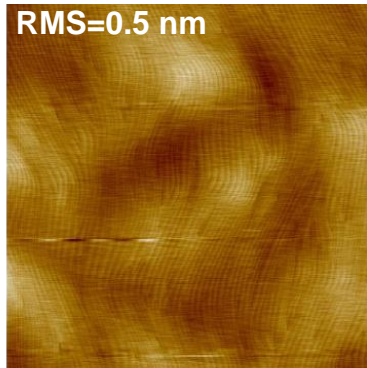
Deliv n.	Title	Delivery month	Partner in charge	Status
D5.1	Project website	M3 (31 July 2020)	<b>CNR</b> , all	<b>Done</b>
D4.1	Data Management Plan	M5 (30 Sept 2020)	<b>CNR</b> , all	<b>Done</b>
D5.2	Plan for Dissemination	M12 (31 March 2021)	<b>U-Pa</b> , all	<b>In prep</b>
D1.1	Report on the growth and surface preparation of hexagonal WBG substrates	M12 (31 March 2021)	<b>CNRS</b>	<b>In prep</b>
D4.2	1st Progress Report	M12 (1 April 2021)	<b>CNR</b> , all	<b>In prep</b>

# Preparation of WBG substrates for TMD deposition

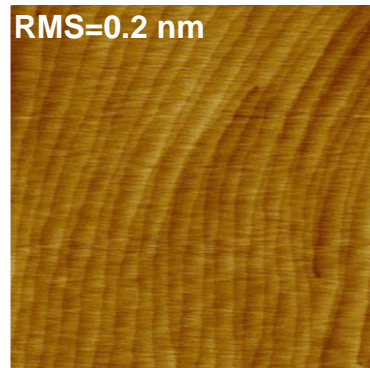


- III-N templates (GaN, AlN and AlGaIn) grown by MOCVD or MBE
- Preliminary characterization by AFM, XRD, XPS

## 3.5 $\mu\text{m}$ GaN/Sapphire



2  $\mu\text{m}$



0.5  $\mu\text{m}$

Dislocation density

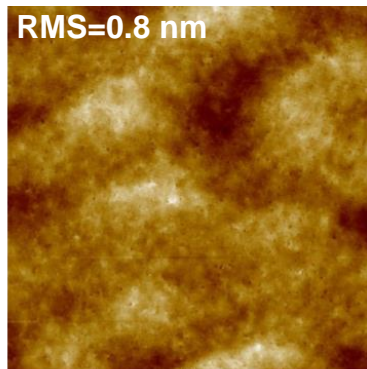
$$\sim 3 \times 10^8 \text{ cm}^{-2}$$

FWHM on XRD rocking curves:

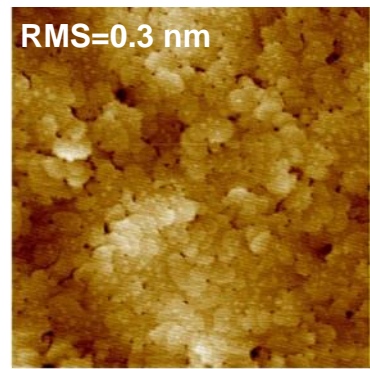
$$\text{GaN (002)} = 396 \text{ ''}$$

$$\text{GaN (302)} = 360 \text{ ''}$$

## 100 nm AlN/Si (111)



2  $\mu\text{m}$



0.2  $\mu\text{m}$

Dislocation density

$$\sim 5 \times 10^{10} \text{ cm}^{-2}$$

FWHM on XRD rocking curves:

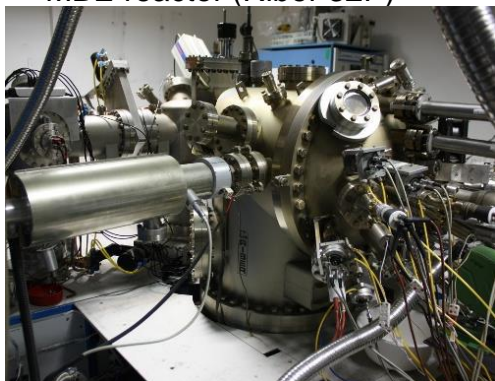
$$\text{AlN (002)} = 2880 \text{ ''}$$

$$\text{AlN (103)} = 3350 \text{ ''}$$

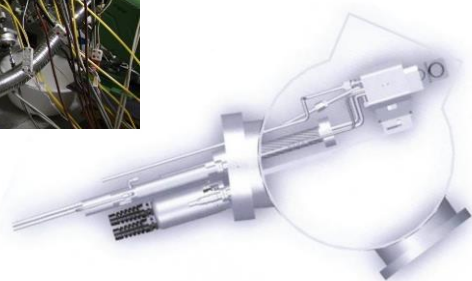
# Molecular Beam Epitaxy of TMDs



MBE reactor (Riber 32P)



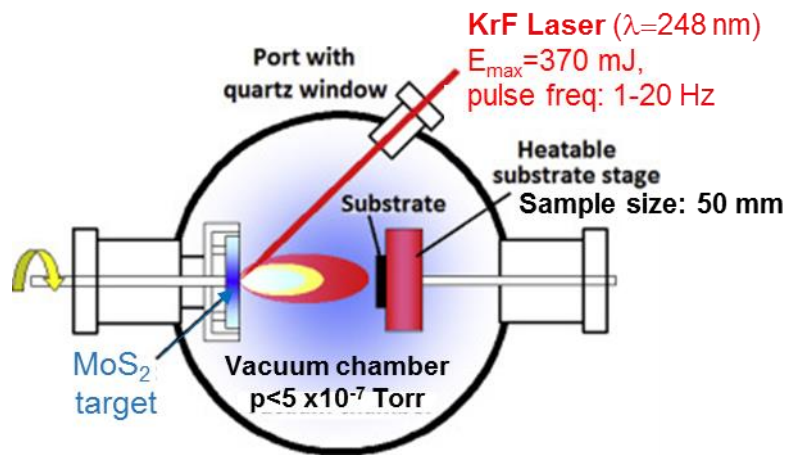
- MBE growth of MoS<sub>2</sub> and WSe<sub>2</sub> in progress
- Preliminary characterization by AFM, XRD, XPS



- Order and installation e-beam evaporators for Mo and W.
- Design and order for the H<sub>2</sub>S gas line



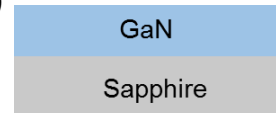
# Pulsed Laser Deposition of MoS<sub>2</sub>



(i) **Substrates**



(ii)



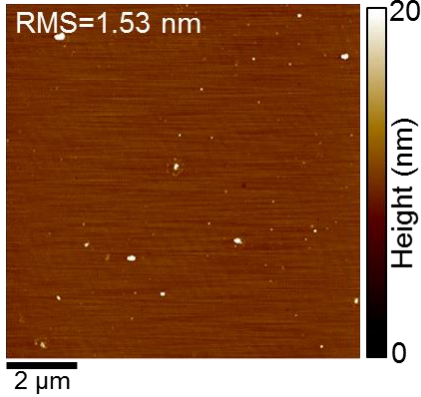


# Development of PLD process on sapphire

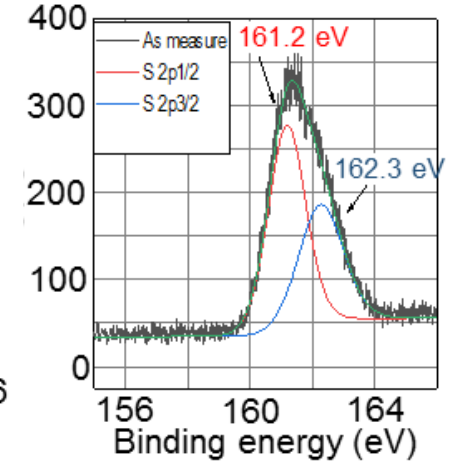
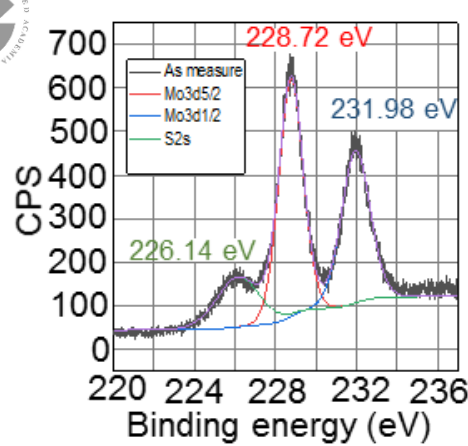
MoS<sub>2</sub>  
Sapphire



**AFM**  
Very flat surface



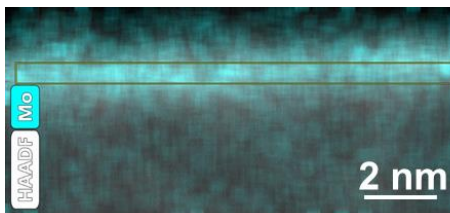
**XPS** Stoichiometry [Mo]:[S]=1:2



**TEM**

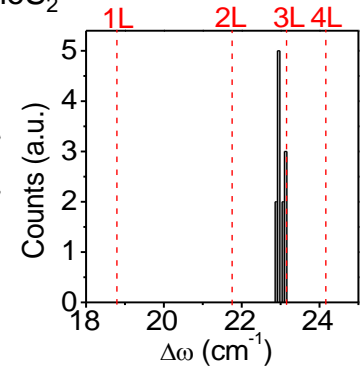
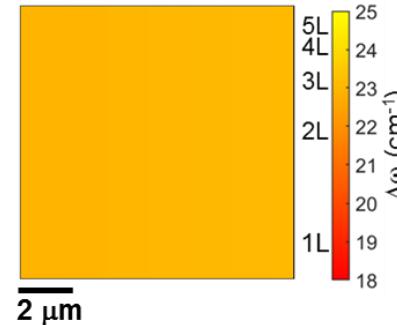
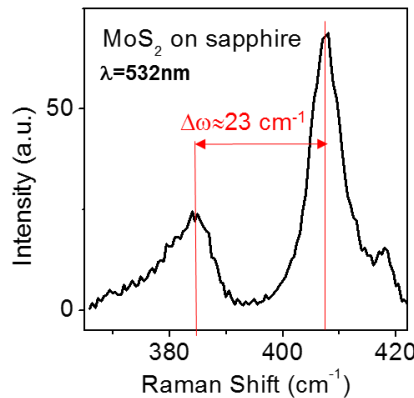


**STEM-HAADF**

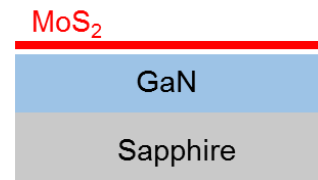


**Micro-Raman mapping**

Very uniform coverage with 3L MoS<sub>2</sub>

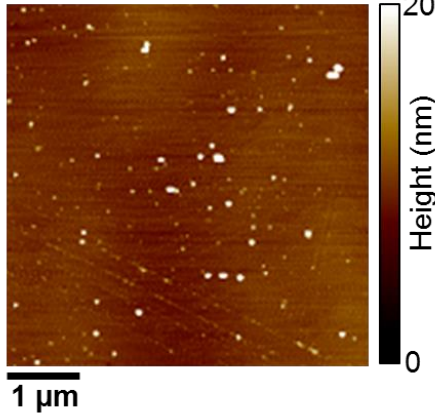


# PLD of MoS<sub>2</sub> on GaN-on-sapphire



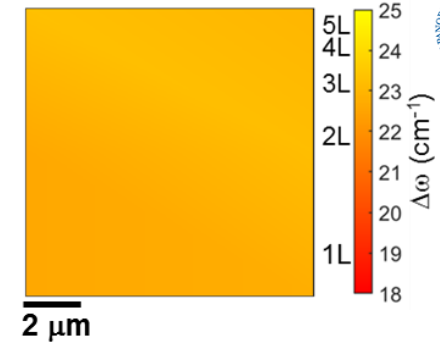
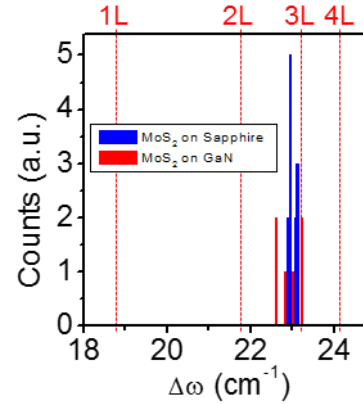
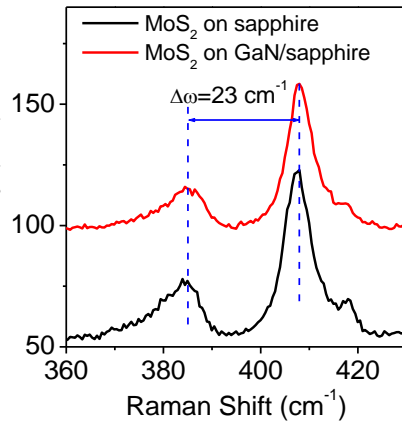
AFM

RMS=1.6 nm



## Raman mapping

Very uniform 3L-MoS<sub>2</sub>



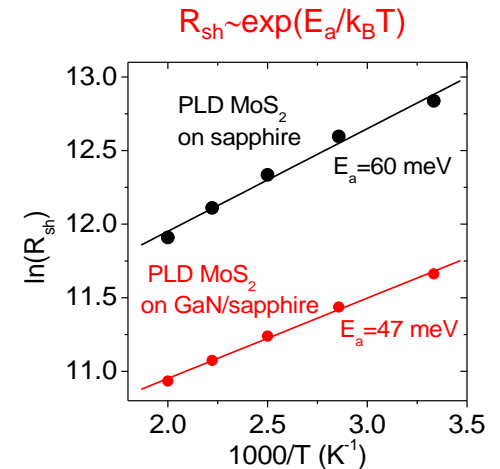
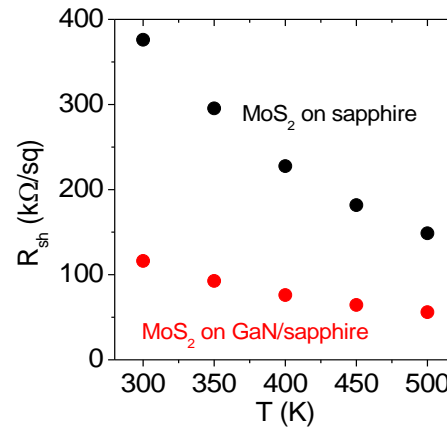
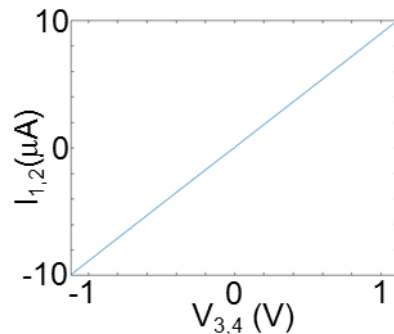
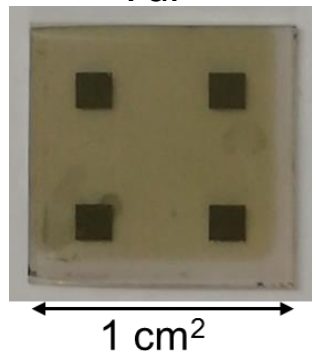
## Electrical characterization

Temperature dependent sheet resistance measurements

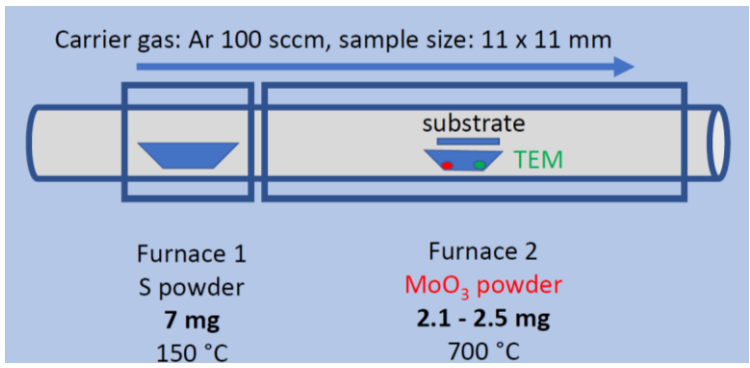


VdP

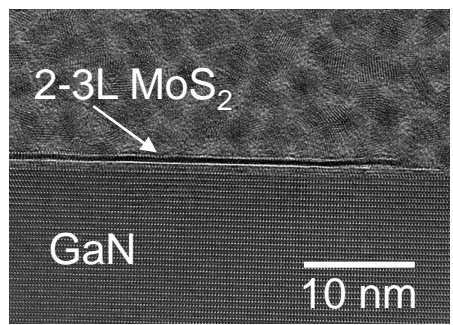
Ni (20 nm)/Au(80 nm) Ohmic contacts onto MoS<sub>2</sub>



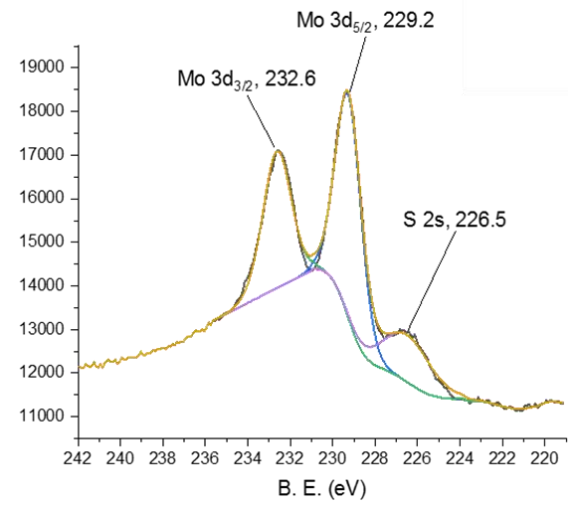
## CVD from S and MoO<sub>3</sub> powders



## HRTEM

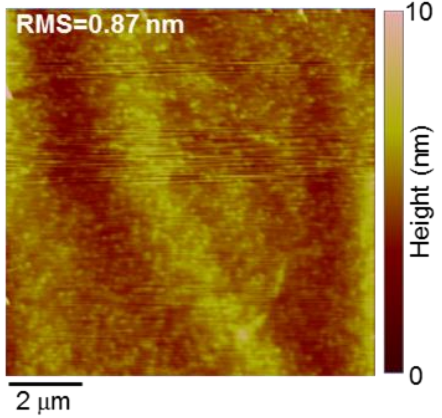


## XPS Stoichiometry [Mo]:[S]=1:1.9



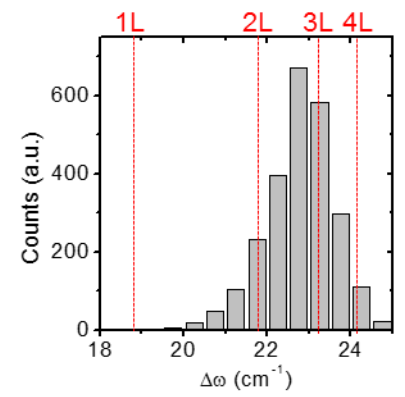
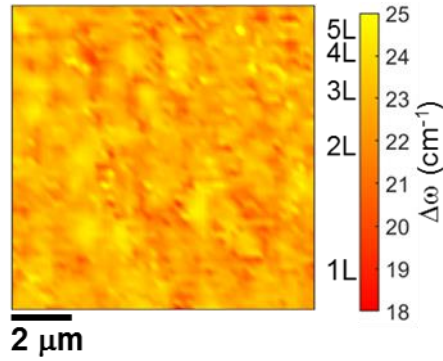
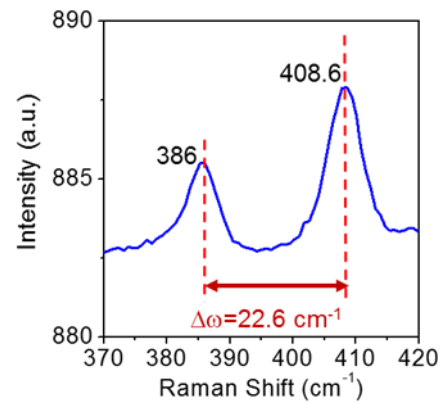
## AFM

Very smooth surface



## Raman mapping

MoS<sub>2</sub> thickness from 2L to 4L



# Management

## Project meetings:

- 1<sup>st</sup> online ETMOS meeting with all partners: 16 June, 2020
- 2<sup>nd</sup> online ETMOS meeting with all partners: 15 December, 2020
- Monthly updates about progress in joint experiments between involved partners

## Association of ETMOS to the Graphene Flagship



### Memorandum of Understanding (MoU)

#### *for association of a Partnering Project to the Graphene Flagship*

Following the submitted application and the approval by the Graphene Flagship Management Panel, the project:

**Epitaxial Transition Metal dichalcogenides Onto wide bandgap hexagonal Semiconductors  
for advanced electronics**

(ETMOS)

becomes associated to the Graphene Flagship initiative as a Partnering Project (PP).

The following organisations shall be granted the status of **Associated Member**:

**Slovak Academy of Sciences, Slovenia (new PI)<sup>2</sup>**

**Università degli Studi di Palermo, Italy**

On behalf of the Graphene Flagship Core 3  
Project:

WP1 Leader  
Vladimir Falko  
Name and signature:

Professor Vladimir Falko, Director of National Graphene Institute, University of Manchester, email: v.falko@manchester.ac.uk, ctd@ Date: 2020.02.20 14:13:59 Z

On behalf of the Partnering Project:

PP coordinator  
Filippo Giannazzo  
Name and signature:

A handwritten signature in blue ink, appearing to read "Filippo Giannazzo".

**Consortium Agreement:** signed by all partners on 17 October 2020;  
sent to FLAG-ERA Secretariat on 23 October 2020

# Dissemination

**ETMOS website** (*available since July 2020*)

- Information on ETMOS consortium and scientific activities
- Dissemination of project results (publications)
- Videos of presentations
- Organized events (symposia, seminars)
- Links to FLAG-ERA and Graphene Flagship events

Home Summary & Keywords Participants Meetings Publications Events Links Contacts Restricted area

**ETMOS**  
Epitaxial Transition Metal dichalcogenides Onto wide bandgap hexagonal Semiconductors for advanced electronics

**FLAG-ERA Workshop 2021**  
March 16<sup>th</sup>-18<sup>th</sup>, 2021

**ETMOS project results presented at**  
Nanoscientific Symposium China 2020,  
Scanning Probe Microscopy  
December 10<sup>th</sup>, 2020  
Presentations available [HERE](#)

 FLAG-ERA

**Joint Transnational Call (JTC) 2019**  
Project  
**ETMOS**  
Epitaxial Transition Metal dichalcogenides Onto wide bandgap hexagonal Semiconductors for advanced electronics

# Dissemination

- **SPECIAL ISSUE** of Nanomaterials on “Nanoscale Electrical Characterization of Low Dimensional Materials for Electronics”, Eds. Giannazzo, Celano
- **BOOK CHAPTER:** F. Giannazzo, E. Schilirò, R. Lo Nigro, P. Prystawko, Y. Cordier, Integration of 2D materials with nitrides for novel electronic and optoelectronic applications, Ch. 11 of *Nitride Semiconductor Technology: Power Electronics and Optoelectronic Devices* ed F Roccaforte and M Leszczynski (Weinheim: Wiley-VCH Verlag). pp 397–438

## Publications:

1. E Schilirò, R Lo Nigro, SE Panasci, FM Gelardi, S. Agnello, Rositsa Yakimova, F Roccaforte, F Giannazzo, *Aluminum oxide nucleation in the early stages of atomic layer deposition on epitaxial graphene*, Carbon **169**, 172-181 (2020).
2. F Giannazzo, R Dagher, E Schilirò, SE Panasci, G Greco, G Nicotra, F Roccaforte, S Agnello, J Brault, Y Cordier, A Michon, *Nanoscale structural and electrical properties of graphene grown on AlGaN by catalyst-free chemical vapor deposition*, Nanotechnology **32**, 015705 (2020)
3. F. Giannazzo, E. Schilirò, G. Greco, F. Roccaforte, *Conductive Atomic Force Microscopy of Semiconducting Transition Metal Dichalcogenides and Heterostructures*, Nanomaterials **10**, 803 (2020)

## Conference Talks (invited):

1. F. Giannazzo, et al., *Nanoscale probing the electronic transport in transition metal dichalcogenides by conductive atomic force microscopy*. NanoInnovation 2020, Roma, 16 September 2020 (online).
2. F. Giannazzo, et al., *2D materials heterojunctions with Nitride semiconductors: from synthesis to applications*, ICTF-JVC 2020 online conference, Budapest, 24 November 2020 (online).
3. F. Giannazzo, et al., *Conductive Atomic Force Microscopy of 2D Materials and Heterostructures for Nanoelectronics*, Nanoscientific Symposium China, 10 December 2020 (online).
4. S. Agnello, et al., *Graphene and transition metal dichalcogenides: from structural properties to doping*, SIF conference, 18 September 2020 (online).
5. Š. Chromik et al., *The properties of  $\text{MOS}_2$  two-dimensional system prepared by PLD and ex-situ methods on different substrates*, 11th International Conference on Solid State Surfaces and Interfaces, Smolenice, Slovakia, 23-26 November 2020.

# Responsible Research Innovation (RRI) in the ETMOS project

## Science Education

- Direct involvement of PhD students in the project's activity
- Organization of dedicated initiatives for **secondary schools and university students** in collaboration with teachers: laboratory visits, experimental demonstrations and training,...

## Public engagement

- Participation to public events (e.g., “**European Researchers' Night**”) with specific activities aimed at illustrating the societal and environmental benefits of new technologies based on advanced materials (2D materials, WBG semiconductors)
- Use of broad audience channels (interviews in newspapers/magazines, dedicated web pages in social networks Facebook, LinkedIn) to disseminate relevant project's achievements.

## Engagement of stakeholders

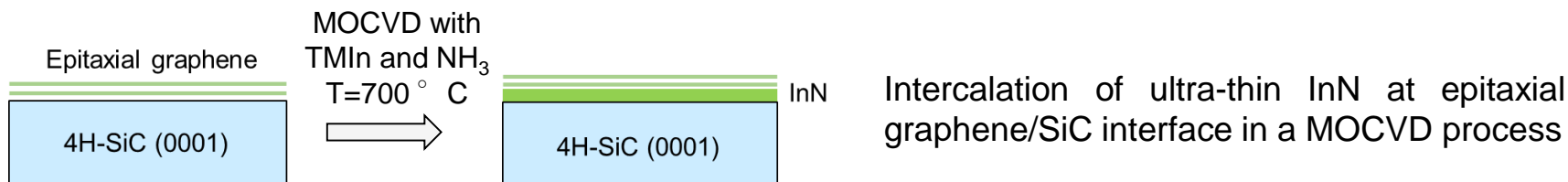
- The CNR-IMM and CNRS-CRHEA partners of ETMOS are involved in National and EU projects on WBG semiconductors (SiC, GaN) with leading **microelectronic industries**, such as **STMicroelectronics** (Italy and France) and small medium enterprises, such as **TopGaN** (Poland).
- Representatives of these industries are involved as **ETMOS Advisory Board Members**, providing guidelines for the compatibility of processes developed in the project with industrial requirements.
- Organization of dedicated seminars/meetings for potential industrial end-users, with the assistance of the advisory board members.

# Interaction with other FlagERA projects

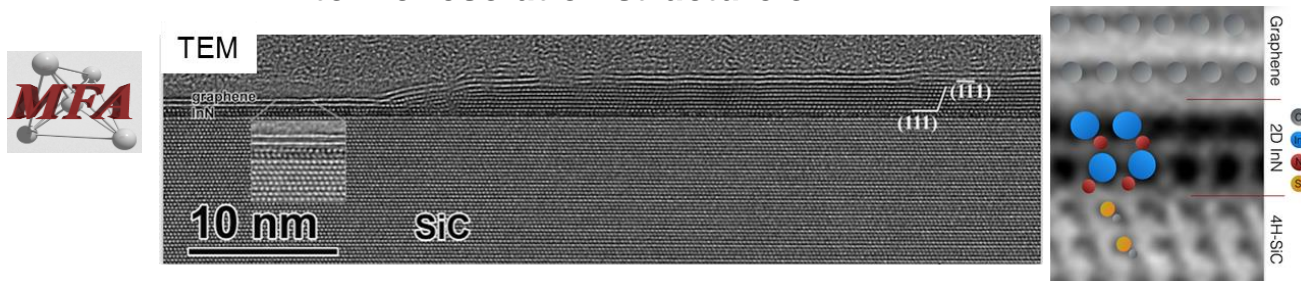


**FLAG-ERA JTC 2015 GRIFONE** (coord. A. Kakanakova-Georgieva, Univ. Linköping, Sweden)

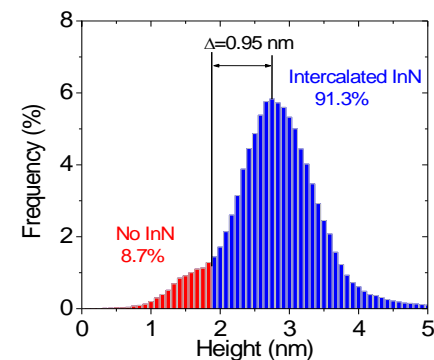
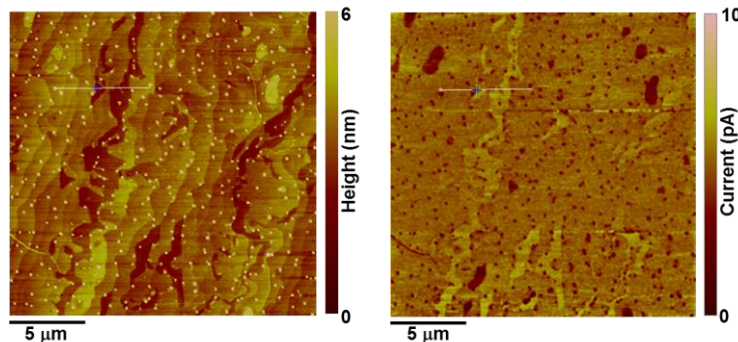
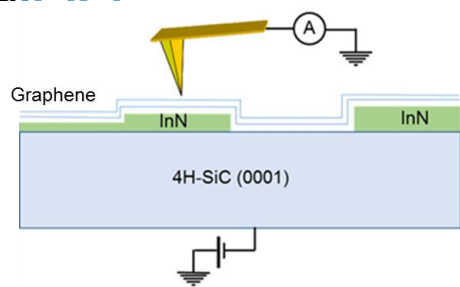
## Nitride semiconductors (InN, AlN, GaN) at the 2D limit



### Atomic resolution structure of 2D-InN



### Uniformity of intercalated 2D-InN



B. Pécz, G. Nicotra, F. Giannazzo, R. Yakimova, A. Koos, A. Kakanakova-Georgieva, *Indium nitride at the 2D limit*, *Advanced Materials* **33**, 2006660 (2021).





## Summary

- Scientific activities of ETMOS project are almost on schedule after the first year:
  - *Activities on WBG substrates preparation and characterization completed*
  - *Running activities on MBE and PLD growth on TMDs and their characterization*
- Dissemination of project results through papers' publications and participation to online conferences
- Successful interaction with another FlagERA project: GRIFONE
- RRI in ETMOS: dissemination to general public; interaction with industrial stakeholders

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