

GOALS

GROUPS

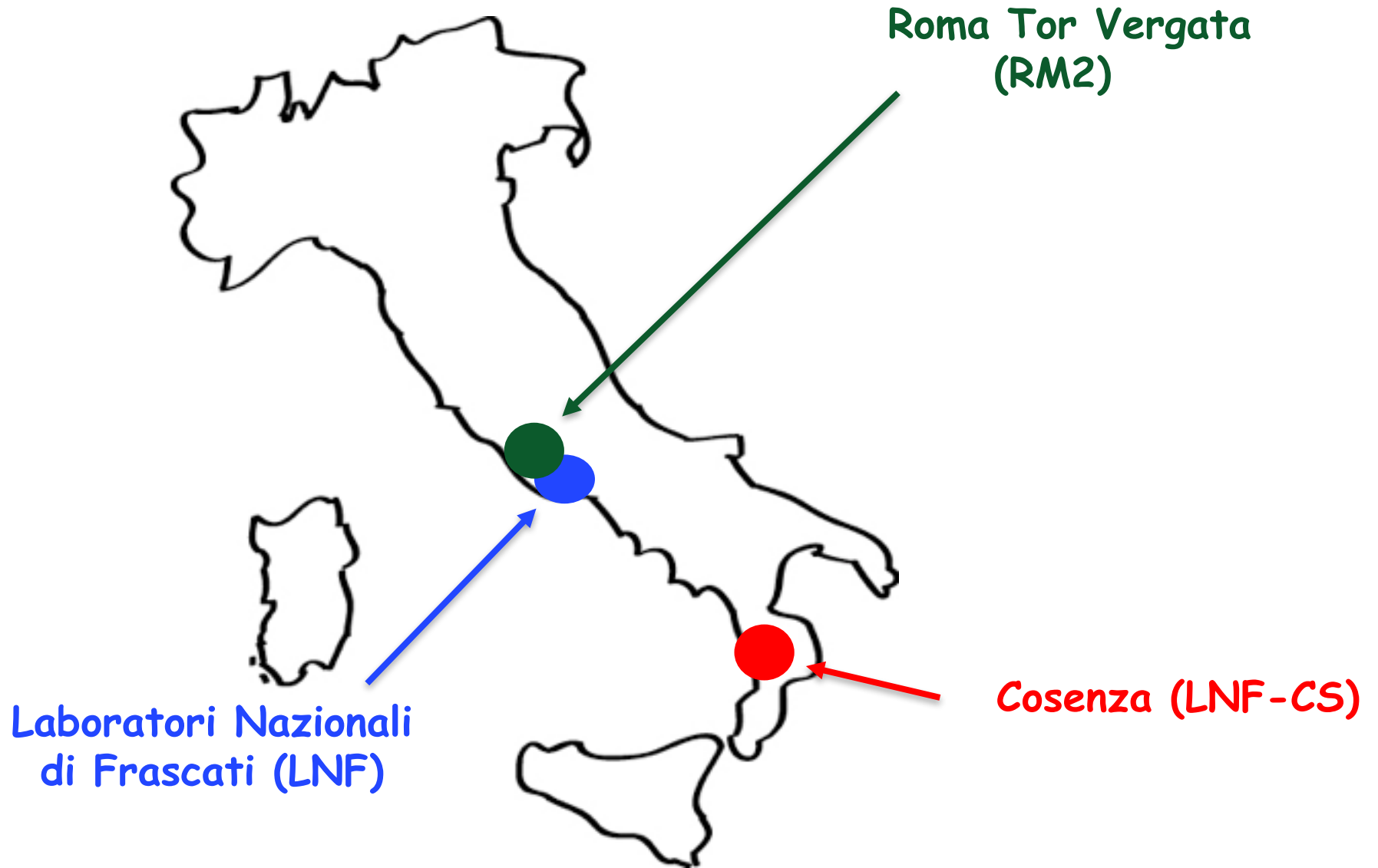
NODIW Proposal

**New Optoelectronic Devices
Integrating 2D materials
in van der Waals
heterostructures**

Methodology

**TIMELINE/
Budget**

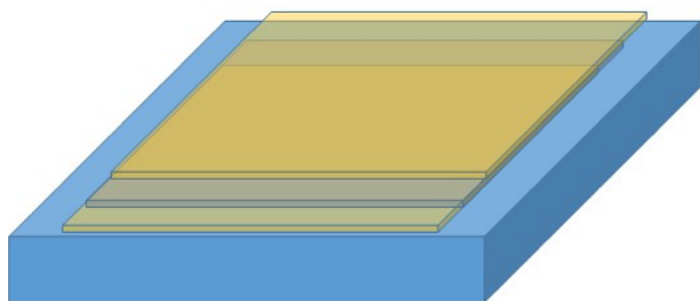
GROUPS



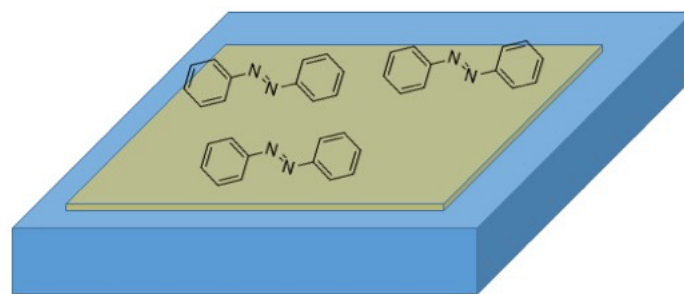
Goals

opto-electronic properties of 2D layered materials (2DLMs) to create novel Van der Waals Heterostructures (vdWHs), which will lead to a new generation of building blocks for device design

(IR photo-detectors, LED, photovoltaics)



Inorganic
vdWHs

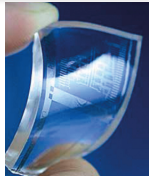


Hybrid vdWHs
Switchable photocromic molecules
/Straintronics

2DLMs: Graphene, MoS₂, MoSe₂, MoTe₂, WS₂, WSe₂ and WTe₂

Why 2D layered materials?

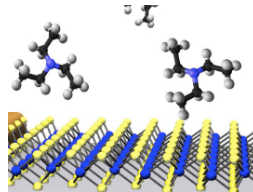
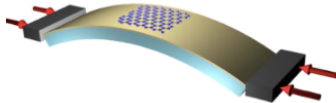
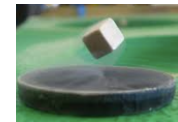
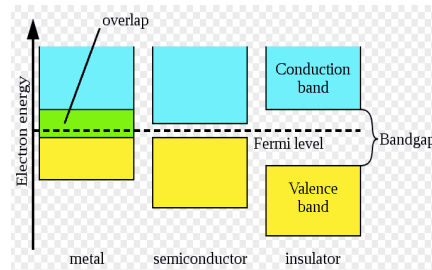
Perfect platform for fundamental physics study and as Building blocks nanoscale devices



Atomic thickness offers
Highly mechanical flexibility
& Large Breaking strengths

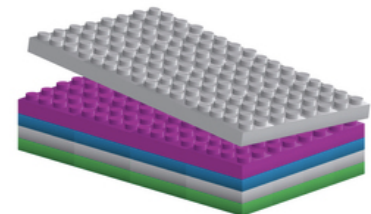
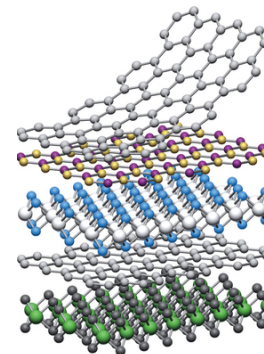


Large variety of
chemical/physical
properties

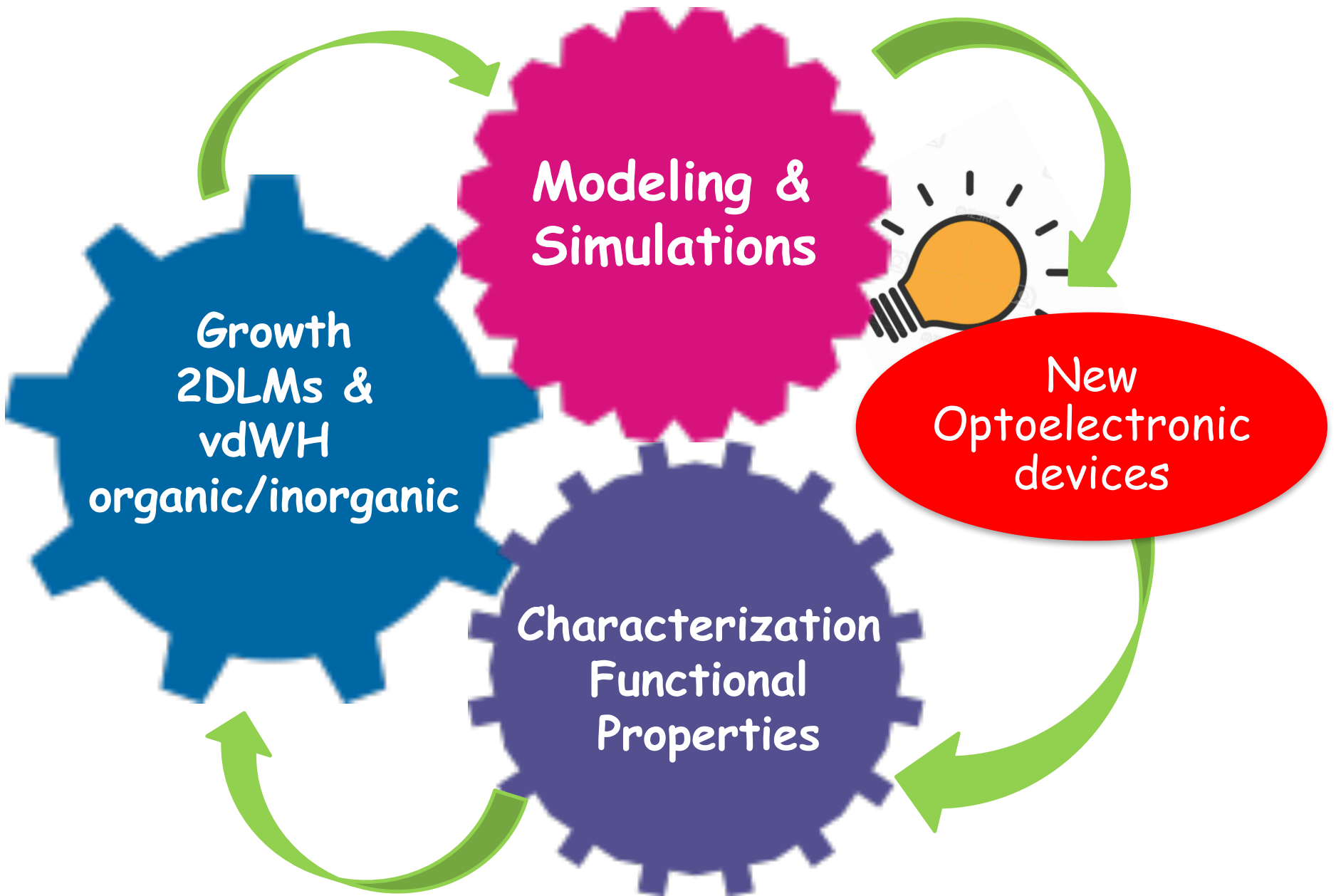


Extremely sensitive to external stimuli:
chemical modification, electric fields
strain deformation, doping

High degree of freedom from
Van der Waals Heterostructuring
to build new functional materials

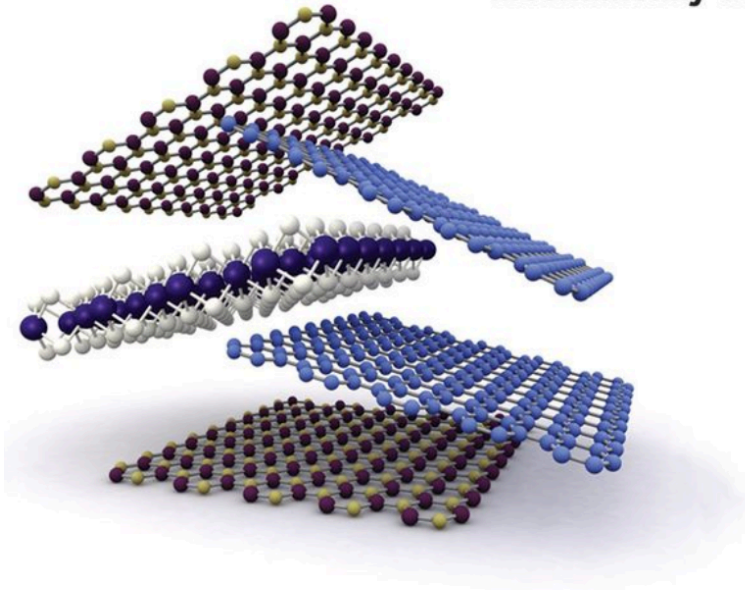


Methodology

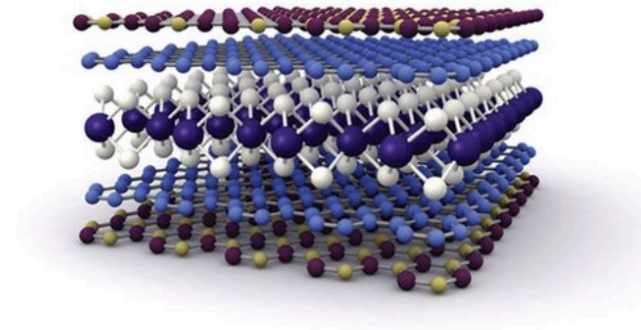


Growth of 2DMLs & vdWH

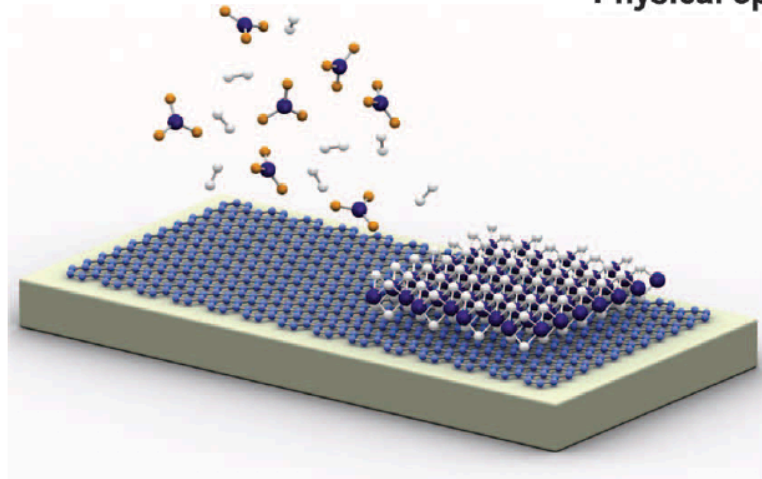
Mechanically-assembled stacks



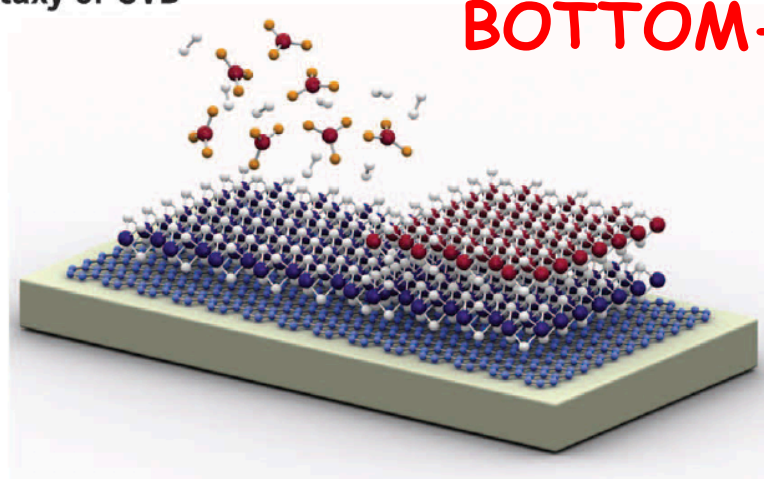
TOP-DOWN



Physical epitaxy or CVD



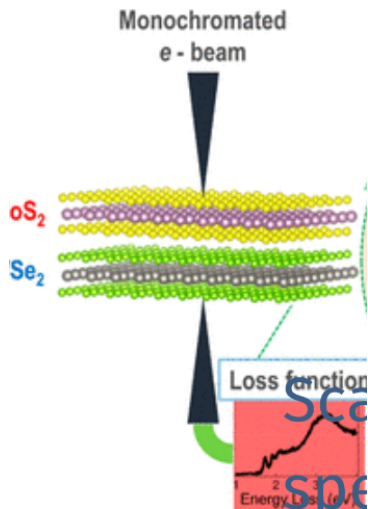
BOTTOM-UP



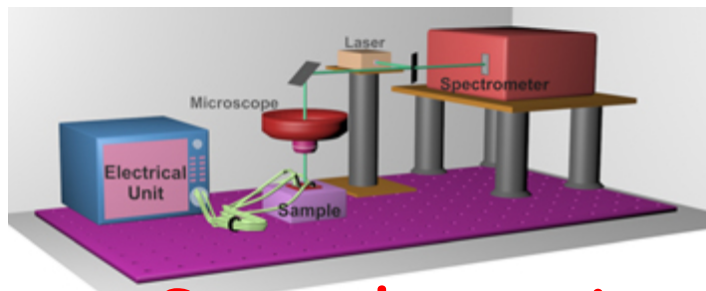
Characterization

PL, RAMAN

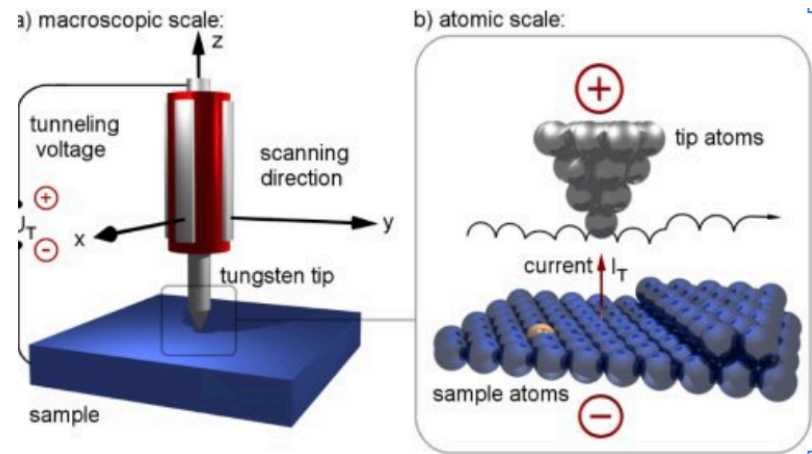
EELS



SEM



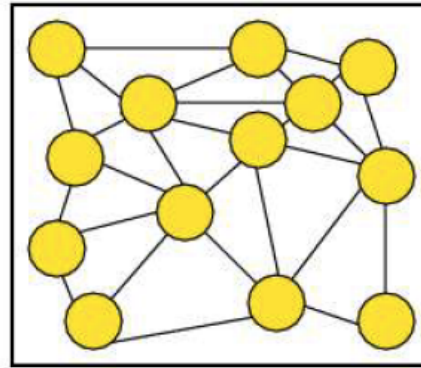
Opto-electronic performances



STM, STS

Modeling & simulations

Fully interacting system



● = particle

Need to describe
ground and excited-state
quantum-mechanical
properties

$$G(r, r', E)$$

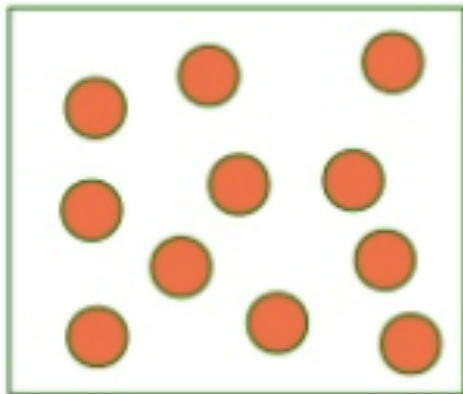
$$n(r)$$

Density Functional Theory

Many-body Perturbation Theory

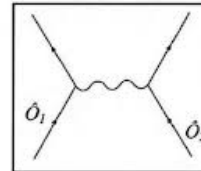


“W. Kohn
Nobel 1998

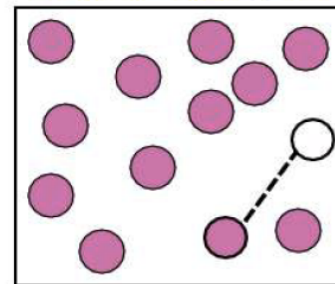


Non Interacting System

FEYNMAN DIAGRAM



Weakly interacting system

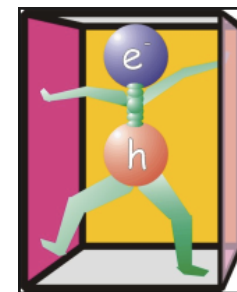


● = Quasiparticle
○ = Quasihole
--- = Screened interaction

GW



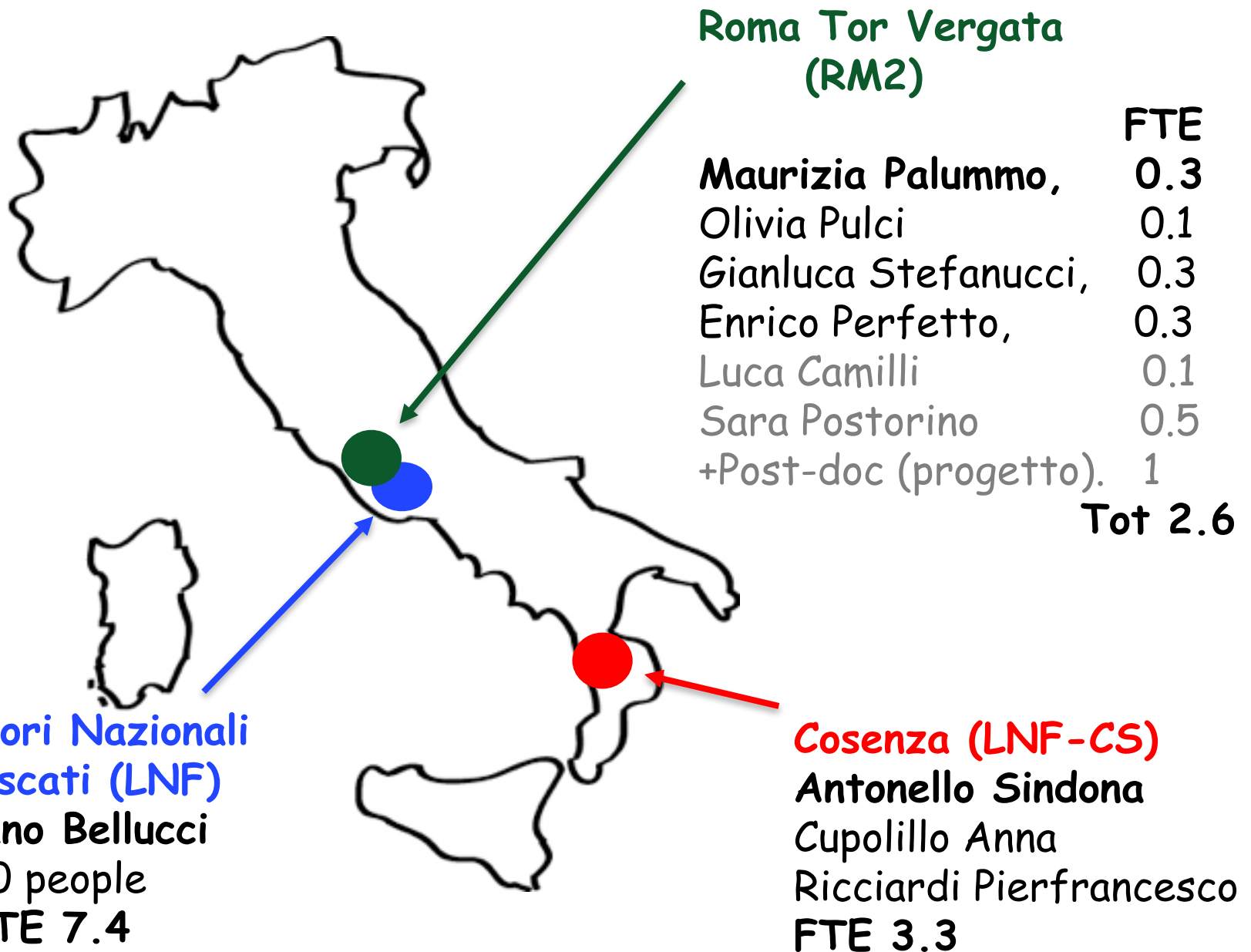
Richard Feynman [1918-1988]



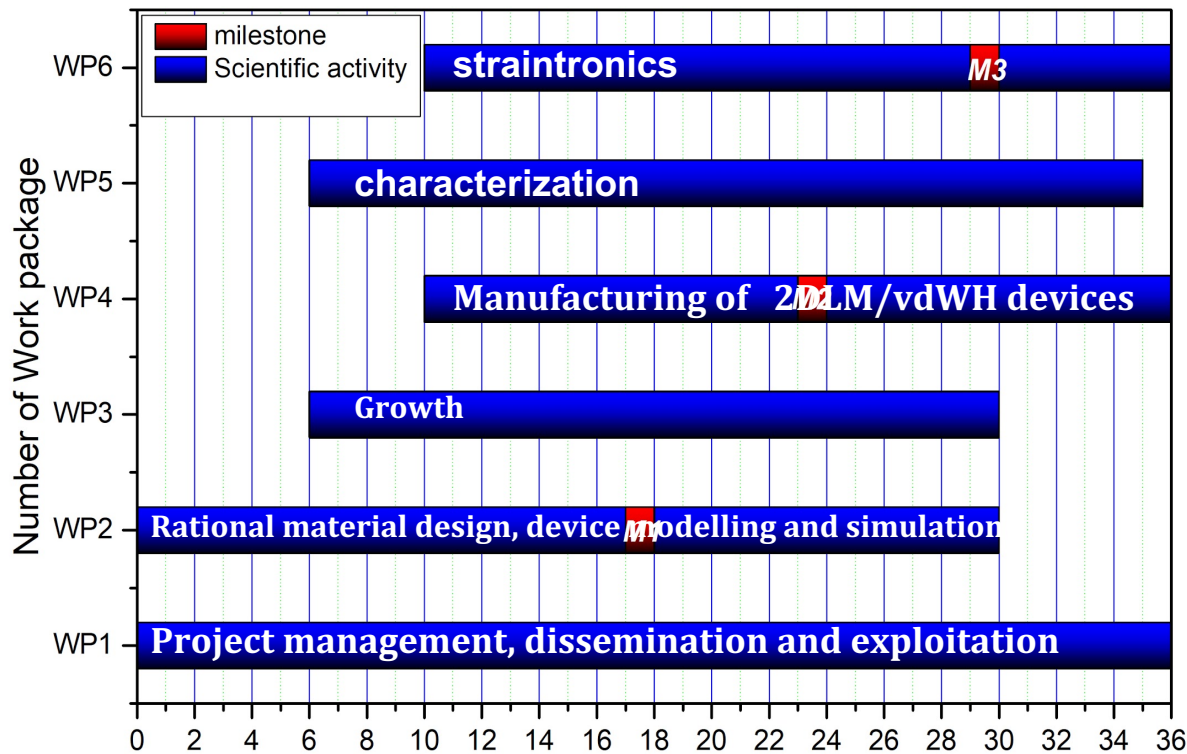
BSE

Excitons

GROUPS



TIMELINE/BUDGET



Budget
Totale
667 keuro

RM2 108
keuro

PREVENTIVO GLOBALE DI SPESA PER L'ANNO 2021

Struttura	A carico dell'I.N.F.N.																			
	missioni		consumo		altri_cons		trasporti		manutenzione		inventario		licenze-SW		apparati		spservizi		TOTALI	
CS	5.00		20.00		24.00														49.00	
LNF	5.00		17.00		30.00				4.00		190.00								246.00	
RM2	10.00		10.00		24.00														44.00	
Totali	20.00		47.00		78.00				4.00		190.00								339.00	

Missioni + pubblicazioni + risorse computazionali + AdR INFN junior



Thank you
for your attention

Modeling & simulations

DFT

Kohn-Sham Equations

$$H_0(r)\varphi_{KS}(r) + v_{xc}(r)\varphi_{KS}(r) = \epsilon_{KS}\varphi_{KS}(r)$$

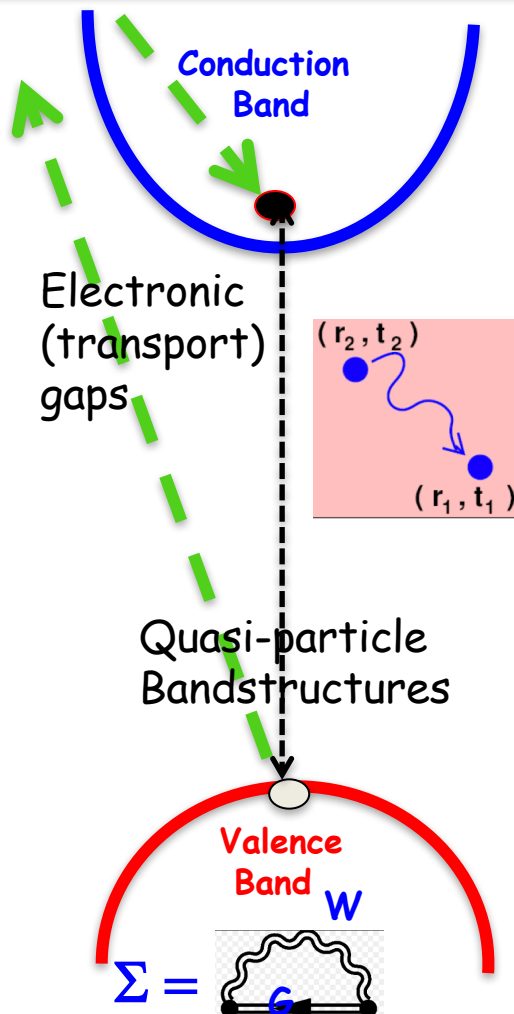


Ground-state properties
KS gaps underestimate
the real QP ones



GW method

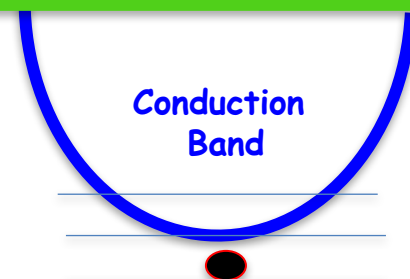
$$\epsilon_i^{QP} \approx \epsilon_i^{KS} + \langle \varphi_i^{KS} | \Sigma(\epsilon_{nk}^{KS}) - V_{xc} | \varphi_i^{KS} \rangle$$



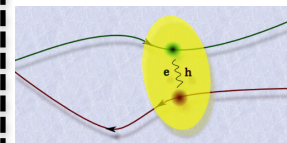
Bethe-Salpeter Equation (BSE)

$$[H_{el} + H_{hole} + H_{el-hole}]A_\lambda = E_\lambda A_\lambda$$

$$Abs(\omega) \propto \sum_\lambda \left| \sum_{vc} A_\lambda^{(vc)} \langle v | D | c \rangle \right|^2 \delta(E_\lambda - \omega)$$



Optical
Gaps,
spectra



A_λ = excitonic eigenfunctions
 E_λ = excitonic Eigenvalues

Modeling & simulations

DFT

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$$H_0(r)\varphi_{KS}(r) + v_{xc}(r)\varphi_{KS}(r) = \epsilon_{KS}\varphi_{KS}(r)$$

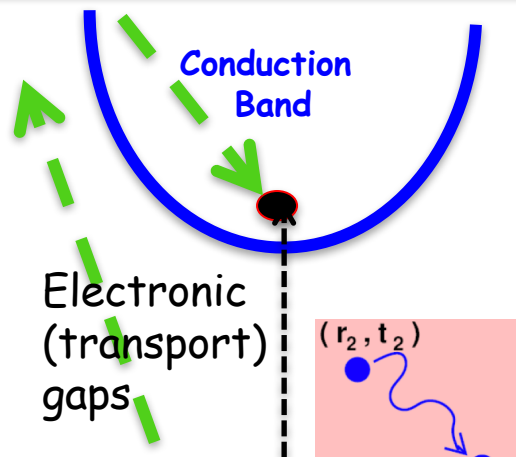


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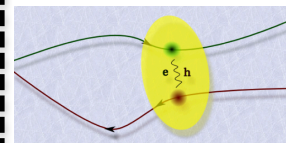
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ABSORPTION,
REFLECTIVITY, EELS,...

Optical
Gaps,
spectra



Valence Band

A_λ = excitonic eigenfunctions
 E_λ = excitonic Eigenvalues