

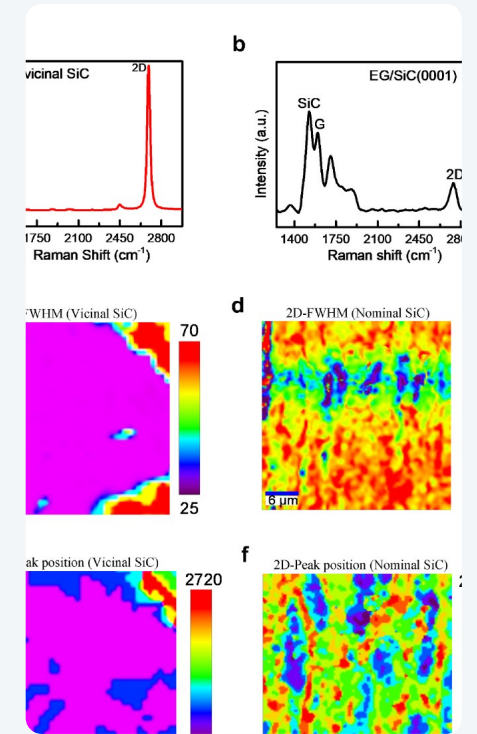
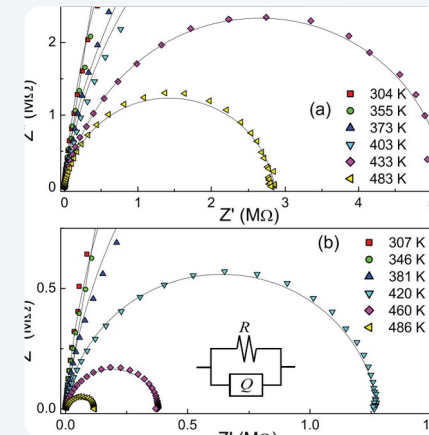
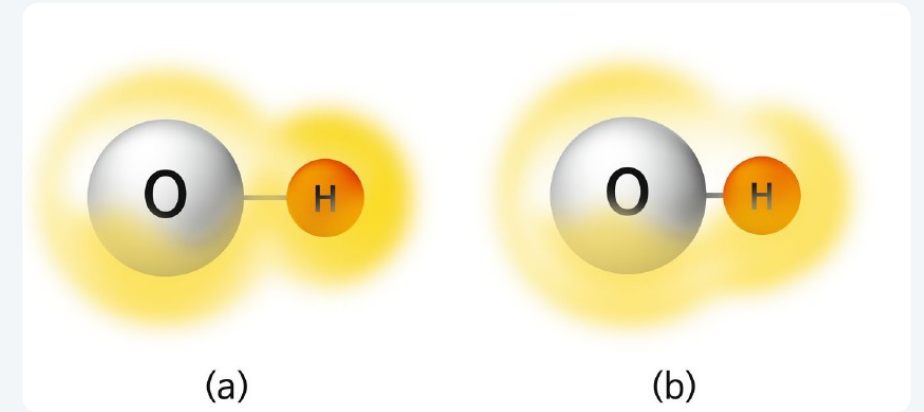
Advanced Materials & Interface De-Risking

From atomistic insight to industrial validation

Prof. Se-Hun Kim

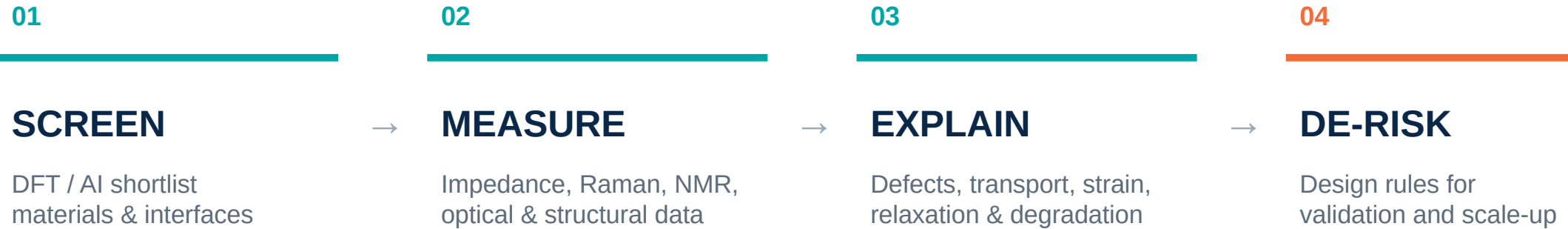
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HORIZON-CL4-2027-01-MAT-PROD-22



I connect computation to experimental proof

I help partners choose materials faster—and explain why they will work.



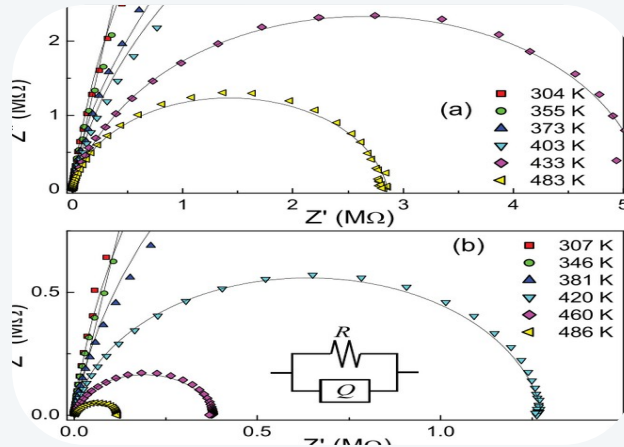
Best consortium position

Scientific partner · Task/WP co-lead

HPC simulation · impedance / ellipsometry
shared XRD · XPS · AFM · FESEM/TEM

Three proven capabilities reduce partner risk

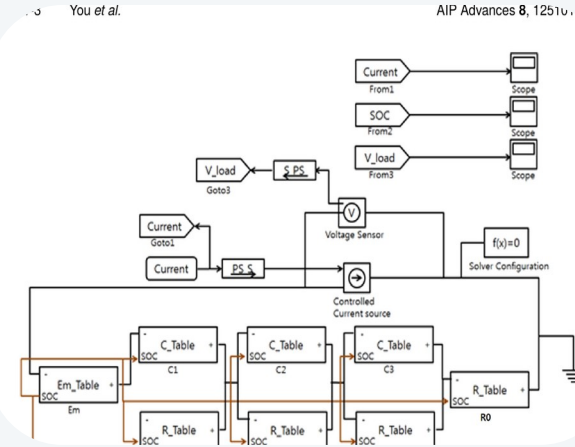
Peer-reviewed evidence across impedance, battery models and graphene devices.



IMPEDANCE

ZnO process effect

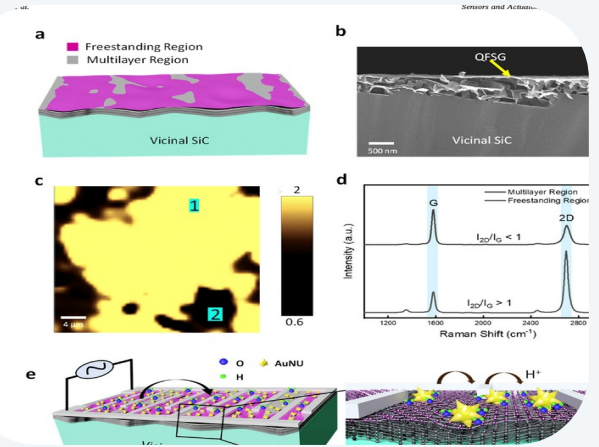
$$\approx 100 \times \sigma \cdot 0.62 \rightarrow 0.30 \text{ eV}$$



BATTERY

3RC model

Lower error than 1RC



SENSOR

Graphene humidity

4–96% RH · 4.5/3.0 s · 25 d

Consortium value: process comparison · model selection · mechanism reports · validation priorities

My contribution maps directly to MAT-PROD-22

Innovative advanced materials and new production processes—reducing dependencies on Critical and Strategic Raw Materials

WHAT THE TOPIC NEEDS

- Substitution or more efficient use of critical / strategic raw materials
- Innovative advanced materials integrated into products and processes
- Performance, safety, sustainability and scalability
- SSbD-guided, transparent decision-making
- Innovation Action pathway: TRL 5 → 7

JNU CONTRIBUTION

- DFT / AI down-selection of CRM-lean material options
- Interface, defect and transport mechanism analysis
- Impedance / Raman / XPS / electrical data interpretation
- Traceable comparison of performance–safety–sustainability trade-offs
- Design rules and evidence package for partner validation

Best fit: scientific partner or Task Lead in an industry-led Innovation Action.

A ready-to-integrate work-package module

Materials & Interface De-Risking by DFT/AI and Advanced Characterization

T1

Screen

Candidate 2D / MXene / interface materials

T2

Explain

Defects, band alignment, charge and ion transport

T3

Validate

Interpret impedance, Raman, XPS and electrical data

T4

De-risk

Recommend stable, scalable combinations

CONSORTIUM OUTPUTS

D1

Candidate database

D2

Screening report

D3

Mechanism report

D4

Interface design rules

D5

Joint technical package

Indicative KPI: screen 20–50 combinations → shortlist 5–10 for partner validation.

Consortium status—and the partners still needed

CURRENT POSITION

Prospective consortium

- JNU, Korea — scientific partner / Task or WP co-lead
- IMNR, Romania — KEREC-matched prospective partner
- NCSR Demokritos, Greece — initial expression of interest
- Status — non-binding; industrial use case still open

WE ARE LOOKING FOR

EU coordinator

Industry-led IA with a clear product / process dependency

Essential partners

Materials / process owner
Pilot-line & end-user validation

Cross-cutting

SSbD · LCA/TEA · circularity
exploitation · scale-up

Three decisions to launch

A focused Brussels conversation

- 01 — Which product or process dependency will we reduce?
- 02 — Who will coordinate—and validate at pilot / end-user level?
- 03 — Where can JNU own a Task or co-lead the materials WP?

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