

MECHANIC

Modelling Charge and Heat transport in 2D-material Composites

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WHO?

CHALMERS
UNIVERSITY OF TECHNOLOGY



P. Erhart

UCL
Université
catholique
de Louvain



J.-C. Charlier



L. Colombo

National Research
Council of Italy



V. Palermo



Izmir Institute
of Technology



H. Sevincli

ICN2

Institut Català
de Nanociència
i Nanotecnològi



S. Roche

avanzare

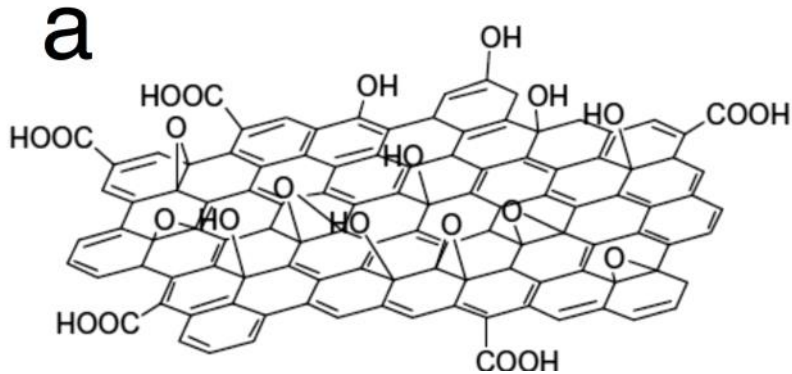
J. Gomez



WHAT and WHY?

Graphene polymer composites ideally inherit properties of functional filler

Electrical and thermal transport **Typically filler is rGO/GO**



Disorder on multiple length scales !

Scalable modeling of heat & charge transport in GO/rGO few layer films with disorder

Experimental verification with FLAG-SHIP core partners

HOW?



J.-C. Charlier



S. Roche

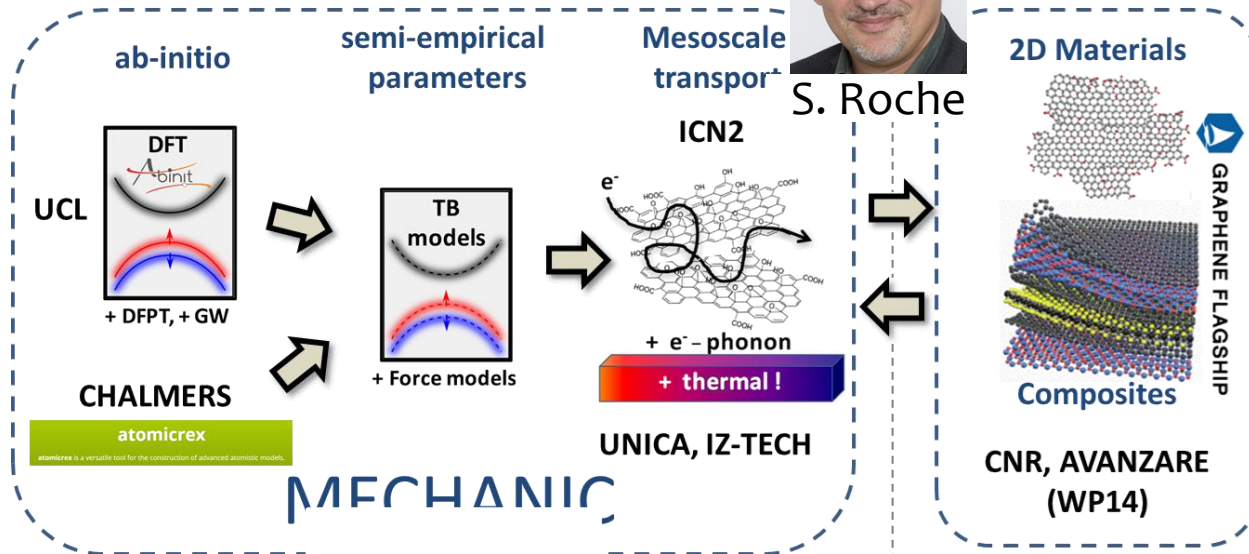
Multi-scale modeling

Synthesis
characterization

Hi-Res TEM
Characterization
of morphology

Transport
measurements

Validation against
produced polymer
composites



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1 Å

10 nm

1 μm

> 10 μm

Length scale

Ab-initio/DFT

Transport + interactions

Order-N transport

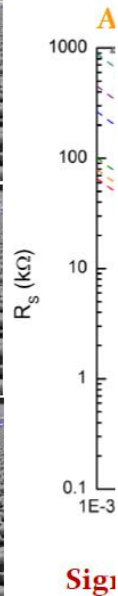
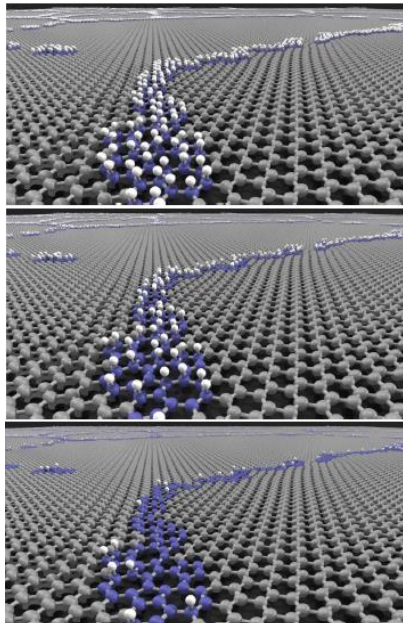
Reality

(AGF/MFT)

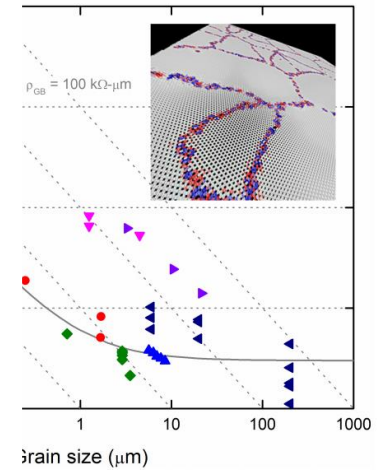
(MD/TB)

TARGETS

MS1 – Demonstrate accurate comparisons between modelling and experiments for scaling properties of charge mobility and thermal conductivity for samples sizes up to $10 \mu\text{m}^2$.



Treat inter-flake transport



General project info

- 4 Partners receiving funding
- 3 partners not funded by FLAG-ERA JTC2017
- **3 Year project** (kick-off meeting 2018-03-14 Bilbao)
- 3 WPs
 - **WP1:** Management, dissemination, database management
 - **WP2:** Ab initio modelling and TB/IF
 - **WP3:** Transport calculations and validation

project-partner	WP1	WP2	WP3	total
1 (CHALMERS)	8	18	6	32
2 (ICN2)	3	2	27	32
3 (UCL)	3	22	11	36
4 (IZ-TECH)	3	2	91	96
5 (UNICA)	3	2	7	12
6 (CNR)	3	0	6	9
7 (AVANZARE)	3	0	4.5	7.5
total	26	46	152.5	<u>224.5</u>