

**FLAG-ERA workshop - MECHANIC, GRANSPORT and GraSage projects**  
Modelling charge and heat transport in GRM - based composites

**Programme**

**Date and time:** Monday, June 28<sup>th</sup>, 2021; 09:30-17:00

**Location:** Zoom

**Link:** <https://zoom.us/j/93083917998?pwd=bEUvZmpwWmYvVU01V3k0M3VFTmFhdz09>

**Meeting ID:** 930 8391 7998

**Passcode:** 517174

<b>09:30 – 10:45</b>	<b>Welcome and introductions</b>	
	<i>Andreas Isacsson and Marie-Alexandra Neouze</i>	Welcome
	<i>Ian Kinloch</i>	WP14 Activities and Future Challenges
	<i>Julio Gómez Cordón</i>	WP15 Activities and Future Challenges
	<i>NN (TBC)</i>	GRANSPORT Project Introduction (TBC)
	<i>Muhammad Maqsood</i>	GraSage Project Introduction
	<i>Andreas Isacsson</i>	MECHANIC Project Introduction
<b>10:45 – 11:00</b>	<b>Break</b>	
<b>Session #1</b>		
<i>Chair: Stephan Roche</i>		
11:00 – 11:45	<i>Andrea Liscio (MECHANIC)</i>	Multiscale Charge Transport in Van der Waals Thin Films. Reduced Graphene Oxide as a Case Study
11:45 – 12:30	<i>Marjan Maček (GRANSPORT)</i>	Recent progress in simulation of graphene-based devices
<b>12:30 – 13:15</b>	<b>Lunch</b>	
<b>Session #2</b>		
<i>Chair: Jean-Christophe Charlier</i>		
13:15 – 14:00	<i>David Seveno (GraSage)</i>	Heat transport in polyamide-6/graphene nanocomposite at the nanoscale
14:00 – 14:45	<i>Hâldun Sevinçli (MECHANIC)</i>	Charge Transport Simulations in Multilayer Reduced Graphene Oxides

<b>14:45 – 15:00</b>	<b>Break</b>	
<b>Session #3</b>		
<i>Chair: TBA</i>		
15:00 – 15:45	<i>Aleandro Antidormi (MECHANIC)</i>	Atomistic Modelling of Reduced Graphene Oxide and Other Forms of Disordered Graphene
15:45 – 16:15	Ivan Ado (GRANSPORT)	Alternative to Dzyaloshinskii-Moriya interaction for monolayer Fe <sub>3</sub> GeTe <sub>2</sub> and other two-dimensional ferromagnets with trigonal prismatic symmetry
16:15 – 16:45	<i>Fredrik Eriksson (MECHANIC)</i>	Highly anisotropic thermal conductivity in randomly rotated stacks of MoS <sub>2</sub>
16:45 – 17:00	<i>Ana-Maria Ciubotaru (ESF)</i>	Collaboration Opportunities within the Flagship

### Speakers

Aleandro Antidormi - Catalan Institute of Nanoscience and Nanotechnology (ICN2), Spain

Julio Gómez Cordon - Avanzare, Spain (Deputy WP leader of Graphene Flagship WP15)

Ana-Maria Ciubotaru, European Science Foundation (ESF), France

Fredrik Eriksson - Department of Physics, Chalmers University of Technology, Sweden

Andreas Isacsson - Department of Physics, Chalmers University of Technology, Sweden

Ian Kinloch - University of Manchester (Deputy WP leader of Graphene Flagship WP14)

Andrea Liscio, CNR - Institute for Microelectronic and Microsystems (IMM), Italy

Marjan Maček - CEA Grenoble, IRIG-PHELIQS / Université Grenoble Alpes, France

Muhammad Maqsood - AMIBM, Maastricht University, Netherlands

Boris Narozhny - Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology, Germany

Marie-Alexandra Neouze - French National Research Funding Agency, Coordinator FLAG-ERA

David Seveno - Department of Materials Engineering, KU Leuven, Leuven, Belgium

Hâldun Sevinçli - Izmir Institute of Technology, Turkey

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