

LAVOISIER discussions on “Quantum Simulation”

May 8-9 2019

Location: ICN2 (Bellaterra, Barcelona)



“LAVOISIER discussions will focus on exchange about recent progress and challenges in modelling “exciton physics, thermal transport/thermoelectric and magnetic/spin proximity effects”. The participants will address recent advances in modelling excitons in two-dimensional materials, as well as the study of thermal transport and thermoelectrics in graphene and van der Waals heterostructures. The modelling and impact of proximity effects between magnetic, strong spin-orbit coupling and other 2D materials will be also the focus of the meeting.”

Wednesday May 8

Morning

11h30 – opening/presentation of the LAVOISIER discussions

Annick Loiseau, Jean-Christophe Charlier, Matteo Calandra and Stephan Roche

12h-13h **Bernard Urbaszek** (INSA Toulouse)

“Physics of Excitons in 2D materials: advances and questions”

13h-13h30 open discussion (Moderators: **Francois Ducastelle & Annick Loiseau**)

13h30-14h30: Lunch

Afternoon

14h30-15h00 **Ludger Wirtz** (University of Luxemburg)

“Excitons in 2D multi-layers: ab-initio and tight-binding perspectives on Davydov-splitting, inter-layer excitons, localized and delocalized excitons, and exciton-phonon interaction”

15h00-15h30 **Elena Cannuccia** (Univ. Tor Vergata)

“Phonon assisted luminescence in hexagonal Boron Nitride”

15h30-16h Open discussion (Moderator: **Maurizia Palummo & Sylvain Latil**)

16h-16h30 Coffee break

16h30-17h **Lorenzo Sponza** (ONERA)

“Coupling ab-initio and semi-empirical methods to take into account the environment of 2D materials”

17h-17h30 **Daniel Varsano** (CNR Inst. Nanoscience)

“Exciton instabilities in monolayer T'-MoS2 and bulk MoS2 under pressure”

17h30-18h **Zeila Zanolli** (ICN2)

“Ab initio exciton & phonon dynamics in Transition Metal Dichalcogenides”

18h-19h Open discussion & poster session (not confirmed yet)

20h Dinner (Barcelona or Hotel UAB Campus (optional))

Thursday May 9

Morning

9h –9h30 Sergio Valenzuela (ICN2)

“Physics of proximity effects in 2D materials-based heterostructures: recent advances and open questions”

9h30 –10h Jaroslav Fabian (University of Regensburg)

“DFT & TB modelling of 2D materials-based heterostructures: recent results and open questions”

10h –10h30 Mairbek Chshiev (CEA)

“Overview on proximity effects and on spin-orbitronic phenomena at ferromagnetic metal/2D material interfaces”

10h30 –11h Open discussion Moderator: J.C. Charlier & Zeila Zanolli

11h00-11h20: Coffee Break

11h20-11h40: **David Soriano** (Radboud University (Nijmegen))

“2D ferromagnetic materials & van der Waals heterostructures”

11h40-12h: **Ramon Cuadrado** (ICN2)

“Magnetic couplings and anisotropies tuned by graphene in magnetic heterojunctions”

12h-12h30: **Simon Dubois** (UCL) *“2D materials-based magnetic tunnelling junctions”*

12h30-13h: **Open discussion Moderator: Matteo Calandra**

13h-14h: Lunch

Afternoon

14h-14h40 **Adrian Bachtold (ICFO)**

“Thermal transport in 2D materials: recent advances and open questions”

14h40-15h10 **Nicola Marzari (EPFL)**

“Modelling thermal transport in 2D materials”

15h10-15h30 Open discussion (Moderator: **Matthieu Verstraete**)

15h30-16h **Thibault Sohier (EPFL)**

“Electron-phonon interactions in gated 2D materials”

16h-16h30 **Klaas-Jan Tielrooij** (ICN2)

“Observing heat spreading of graphene electrons with femtosecond temporal and nanometer spatial resolution”

16h30-17h Coffee Break

17h-17h30 Open discussion, wrap-up and conclusions

Additional submitted contributions

Matteo Calandra (INSP) “*Magnetism and correlation in two dimensional crystals*”
Daniel Solis, **Fatima Ibrahim**, Ali Hallal, X. Waintal and M. Chshiev, “*Proximity magnetoresistance effects in graphene induced by magnetic and multiferroic insulators*”
Ali Hallal, J. Liang , F. Ibrahim, H. X. Yang and M. Chshiev, “*Perpendicular Magnetic Anisotropy and Dzyaloshinskii-Moriya Interaction at Co/2D material interfaces*”

Practical information

LAVOISIER date/place and location

Date: May 8-9 2019

Place: ICN2 (Bellaterra, Barcelona)

<https://icn2.cat/lavoisier-quantum/>

LAVOISIER meeting place - access information

<https://icn2.cat/en/contact>

HOTEL for participants:

Hotel ExE Campus

<https://www.exehotels.com/exe-campus.html>

reservation by email at eventos@hotelexecampus.com

Notes:

Dinner on May 8 will take place at the Hotel

Reservation should mention “LAVOISIER” and be made before March 25

Reimbursement of rooms will be proceeded after meeting ??????????????????

Organisers: The meeting will be framed within the **LAVOISIER discussions** organized by **GDR graphene & nanotubes** network (<http://www.graphene-and-co.org/>) with the support of ICN2 and the European centre of excellence **MaX - Materials design at the Exascale** (<http://www.max-centre.eu/>)

Local organiser **Stephan Roche** (ICN2, stephan.roche@icn2.cat)

Event contact: Ana de la Osa (ICN2 ana.delaosa@icn2.cat)

Other org. **Matteo Calandra** (INSP- Jussieu) & **Jean-Christophe Charlier** (UCL)



<http://www.graphene-and-co.org/>



DRIVING
THE EXASCALE
TRANSITION

<http://www.max-centre.eu>

LIST OF PARTICIPANTS

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