

## Schedule of HeteroNanoCarb-2025

### Monday 13<sup>th</sup> January 2025

15:00/15:30	Departure Bus from Barcelona Downtown/Airport <a href="http://benasque.org/2025heteronocarb/#benasque">http://benasque.org/2025heteronocarb/#benasque</a>
19:30	Arrival Bus to Benasque
20:30	Welcome cocktail

### Tuesday 14<sup>th</sup> January 2025

### Wednesday 15<sup>th</sup> January 2025

### Thursday 16<sup>th</sup> January 2025

8:15 - 8:40	Registration - Badge				
8:40 - 8:45	Remarks - Announcements				
8:45-10:40	Session I	8:55-10:50	Session IV	8:55-10:50	Session VII
10:40-11:15	Coffee Break	10:45-11:15	Coffee Break	10:45-11:15	Coffee Break
11:15-13:10	Session II	11:15-13:10	Session V	11:15-13:10	Session VIII
13:15-18:30	Mini Workshops	13:15-18:30	Mini Workshops	13:15-18:30	Mini Workshops
18:45-20:20	Session III	18:45-20:20	Session VI	18:45-20:10	Session IX
20:20-21:45	Poster session / Cocktail	20:20-21:45	Poster session / Cocktail	21:00-...	Conference Dinner

### Friday 17<sup>th</sup> January 2025

8:00	Departure Bus to Barcelona Airport/Downtown <a href="http://benasque.org/2025heteronocarb/#benasque">http://benasque.org/2025heteronocarb/#benasque</a>
12:45-13:45	Arrival Bus to Barcelona Airport

**Tuesday 14<sup>th</sup> January 2025**

8:15-8:40	Registration/badge	
8:40 – 10:40	Session - I	Chairs: R. Arenal & A. Molina
Invited Speaker	8:45 – 9:20	<i>Hydrogenating single-layer graphene</i> T. Fournier, S. El-Masaoudi, K. Cruz, B. Lassagne, I. Gerber, M. Monthioux, P. Puech, F. Piazza <a href="mailto:monthiou@cemes.fr">monthiou@cemes.fr</a>
	9:20 – 9:35	<i>PFAS removal using fluorinated carbon-based materials</i> Reza Ghanbari, Mohsen Adeli <a href="mailto:m.aadeli@fu-berlin.de">m.aadeli@fu-berlin.de</a>
	9:35 – 9:50	<i>The characteristics of lesser-known moiré patterns: a focus on higher-order patterns</i> Márton Szendrő, P. Vancsó, T. T. Pham, K. Palotás, R. Castelino, M. Bouatou, C. Chacon, L. Henrard, J. Lagoute, R. Sporken, A. Pálinkás, Z. Osváth <a href="mailto:marciarcu@gmail.com">marciarcu@gmail.com</a>
	9:50 – 10:05	<i>Controlled growth of atomically-thin semiconductor films</i> Ariel Ismach <a href="mailto:aismach@tauex.tau.ac.il">aismach@tauex.tau.ac.il</a>
Invited Speaker	10:05 – 10:40	<i>Graphene and layered materials for photonics and optoelectronics</i> Andrea C. Ferrari <a href="mailto:acf26@cam.ac.uk">acf26@cam.ac.uk</a>
10:40 – 11:15		COFFEE BREAK
11:15 – 13:10	Session - II	Chairs: V. Meunier & A.C. Ferrari
Invited Speaker	11:15-11:50	<i>Ab initio modelling of time-resolved angle-photoemission spectroscopy. Understanding ultrafast exciton dynamics in layered materials</i> Alejandro Molina-Sánchez <a href="mailto:alejandro.molina@uv.es">alejandro.molina@uv.es</a>
	11:50-12:05	<i>Light-matter interactions and trion dynamics in WS<sub>2</sub> nanotubes</i> Hila Shalom, V. Kundrať, I. Pinkas, R. Tenne, L. Yadgarov <a href="mailto:hilas@ariel.ac.il">hilas@ariel.ac.il</a>
	12:05-12:20	<i>Determining by Raman spectroscopy the average thickness and N-layer-specific surface coverages of MoS<sub>2</sub> thin films with domains much smaller than spot size</i> Matthieu Paillet, F.W. Klein, J.-R. Huntzinger, D. Voiry, V. Astié, R. Parret, S. Juillaguet, J.-M. Decams, S. Contreras, P. Landois, A.-A. Zahab, J.-L. Sauvajol <a href="mailto:matthieu.paillet@umontpellier.fr">matthieu.paillet@umontpellier.fr</a>
	12:20-12:35	<i>Resonance Raman response of confined carbyne solely driven by anharmonic interactions</i> Emil Josef Parth, A. Corradini, W. Cui, D. Romanin, C. Freytag, C. Schuster, L. Shi, K. Yanagi, M. Calandra, T. Pichler <a href="mailto:Emil.parth@univie.ac.at">Emil.parth@univie.ac.at</a>
Invited Speaker	12:35-13:10	<i>Fullerenes as a playground to search for quantum functionalities in molecular solids</i> Denis Arčon <a href="mailto:denis.arcon@ijs.si">denis.arcon@ijs.si</a>

**Tuesday 14<sup>th</sup> January 2025**

18:45 – 20:20	Session - III	Chairs: A.V. Krasheninnikov & N. Alem
Invited Speaker	18:45-19:20	<p><i>Mapping the defects in transition metal dichalcogenides through high-throughput first principles computations and experiments</i></p> <p>Geoffroy T.F Hautier  <a href="mailto:Geoffroy.T.F.Hautier@dartmouth.edu">Geoffroy.T.F.Hautier@dartmouth.edu</a></p>
	19:20-19:35	<p><i>Sacrificial role of carbon nanostructures in hybrid titanium dioxide photoelectrodes</i></p> <p>Alejandro Ansón-Casaos, Miqueas Pérez-Hernández, Juan Lemos-Chapela, Carlos Martínez-Barón, José Miguel González-Domínguez, Ana M. Benito, Wolfgang K. Maser  <a href="mailto:alanson@icb.csic.es">alanson@icb.csic.es</a></p>
	19:35-19:50	<p><i>Direct visualization of temperature induced phase separation of completely miscible Au-Pd alloy by in-situ TEM</i></p> <p>Abhijit Roy, Simon Hettler and Raul Arenal  <a href="mailto:aroy@unizar.es">aroy@unizar.es</a></p>
	19:50-20:05	<p><i>Characterisation of host-guest interaction of stabilised C<sub>59</sub>N•C[10]CPP complex radicals</i></p> <p>Yuri Tanuma, B. Anézo, G. Kladnik, M. van Midden Mavrič, H.A. Wegner, N. Tagmatarchis, C. Ewels, D. Cvetko, D.Arčon  <a href="mailto:Yuri.Tanuma@ijs.si">Yuri.Tanuma@ijs.si</a></p>
	20:05-20:20	<p><i>Compositional profiles of the PCBM fullerene derivative with the active layer of organic solar cells</i></p> <p>A. Urbina  <a href="mailto:antonio.urbina@unavarra.es">antonio.urbina@unavarra.es</a></p>
20:20-21:45	<i>Poster Session</i>	<b>Cocktail</b>

8:55 – 10:50	Session - IV	Chairs: N. Tagmatarchis & D. Arcon
Invited Speaker	8:55 – 9:30	<i>Testing nanotribology theories on heterogeneous carbon interfaces</i> Dogan Erbahar, Cem Celebi, Ozhan Unverdi, Mete Oztay, Tuana Karakoyun, Eftal Gezer, D. Ickecan, Semran Ipek, Cicek Kaplan <a href="mailto:derbahar@dogus.edu.tr">derbahar@dogus.edu.tr</a>
	9:30 – 9:45	<i>Fullerene-like C<sub>59</sub>N qubits on diamond substrates. Simulation and experimental development.</i> Bastien Anézo, Yuri Tanuma, Z. Gosar, Denis Arcon, C. Ewels. <a href="mailto:bastien.anezo@ijs.si">bastien.anezo@ijs.si</a>
	9:45 – 10:00	<i>Nonmetallic, bilayer Pt clusters on 2D MoS<sub>2</sub> for ultrafast hydrogen evolution</i> Péter Vancsó, Tamás Ollár, Péter Kun, Antal A. Koós, Ekaterina V. Sukhanova, Zakhar I. Popov, Miklos Németh, Krisztina Frey, Béla Pécz, Péter Nemes-Incze, Chanyong Hwang, József S. Pap, Levente Tapasztó <a href="mailto:vancso.peter@ek.hun-ren.hu">vancso.peter@ek.hun-ren.hu</a>
	10:00 – 10:15	<i>High-throughput calculation of 2D carbon allotropes</i> Vincent Meunier <a href="mailto:vincent.meunier@psu.edu">vincent.meunier@psu.edu</a>
Invited Speaker	10:15 – 10:50	<i>Engineering the structure and properties of 2D materials by defects, strain and intercalation</i> A.V. Krasheninnikov <a href="mailto:a.krasheninnikov@hzdr.de">a.krasheninnikov@hzdr.de</a>
10:50 – 11:15		COFFEE BREAK
11:15 – 13:10	Session - V	Chairs: D. Erbahar & A. Urbina
Invited Speaker	11:15-11:50	<i>Graphene oxide and beyond: Heteronanocarbon structures as functional 2D macromolecular platforms</i> Wolfgang K. Maser and Ana M. Benito <a href="mailto:wmaser@icb.csic.es">wmaser@icb.csic.es</a>
	11:50-12:05	<i>Enhancing structural and electrical properties of semiconducting and insulating nanosheet networks</i> Hannah Wood <a href="mailto:hjw5453@psu.edu">hjw5453@psu.edu</a>
	12:05-12:20	<i>Graphene Oxide @ Enamino-Xanthene Charge Transfer Complexes for TiO<sub>2</sub> Photoelectrode Sensitization</i> Carlos Martínez-Barón, Juan Manuel Garrido-Zoido, Miguel Ángel Álvarez-Sánchez, Alejandro Ansón-Casaos, María Victoria Gil, Ana Benito, Wolfgang Maser <a href="mailto:cmartinez@icb.csic.es">cmartinez@icb.csic.es</a>
	12:20-12:35	<i>Effect of bimetallic catalyst on cellulose-derived graphitic biocarbon for energy applications</i> Shamala Gowri Krishnan, Claire E White, Nandakumar Kalarikkal, Sabu Thomas, Ange Nzihou <a href="mailto:shamala.gowri.krishnan@mines-albi.fr">shamala.gowri.krishnan@mines-albi.fr</a>
Invited Speaker	12:35-13:10	<i>Electron microscopy and spectroscopy of low-dimensional hybrid materials</i> Kazu Suenaga <a href="mailto:suenaga-kazu@sanken.osaka-u.ac.jp">suenaga-kazu@sanken.osaka-u.ac.jp</a>

18:45 – 20:20	Session - VI	Chairs: K. Suenaga & E. Obraztsova
Invited Speaker	18:45-19:20	<i>Controlling functionality in 2D materials: From ferromagnetic and anticorrosive to optoelectronic and bio-applications</i> Mauricio Terrones <a href="mailto:mut11@psu.edu">mut11@psu.edu</a>
	19:20-19:35	<i>Understanding the coupling of graphene oxide with protoporphyrin IX by co-localized Kelvin probe and fluorescence microscopies</i> Víctor Camús, Mario Navarro-Rodríguez, Ana Cros, Núria Garro, Elisa Palacios-Lidón <a href="mailto:victor.camus@uv.es">victor.camus@uv.es</a>
	19:35-19:50	<i>Rheological study of stabilizer blends on rigidity percolation of carbon nanotube dispersions</i> Kevin L. Doty, Alan Dalton <a href="mailto:K.Doty@sussex.ac.uk">K.Doty@sussex.ac.uk</a>
	19:50-20:05	<i>Properties and structural analysis of incommensurate micro- and nano-tubular (Sm<sub>x</sub>Y<sub>1-x</sub>)S-TaS<sub>2</sub> nanotubes based on quaternary misfit layered compounds</i> Mohammad Furqan, Simon Hettler, MB Sreedhara, Reshef Tenne, Raul Arenal <a href="mailto:mfurqan@unizar.es">mfurqan@unizar.es</a>
	20:05-20:20	<i>Engineering friction of 2D materials by defect generation: Graphene and MOS<sub>2</sub></i> Jaime Colchero, Aitor Zambudio, Guillermo López-Polín, Pablo Ares, Julio Gómez-Herrero and Cristina Gómez-Navarro <a href="mailto:colchero@um.es">colchero@um.es</a>
20:20-21:45	Poster Session	<b>Cocktail</b>

Thursday 16<sup>th</sup> January 2025

8:55 – 10:50	Session - VII	Chairs: A. Ismach & M. Monthioux
Invited Speaker	8:55 – 9:30	<i>SWCNT- hybrids confining molecular nanostructures</i> Paola Ayala <a href="mailto:paola.ayala@univie.ac.at">paola.ayala@univie.ac.at</a>
	9:30 – 9:45	<i>2D and 3D Bond mapping in FeO/Fe<sub>3</sub>O<sub>4</sub> nanocubes using the low energy Fe- M<sub>2,3</sub> EELS edge</i> Mario Pelaez-Fernandez, D. del-Pozo-Bueno, M. Marinova, A. Teurtrie, H. Leroux, F. Peiró, S. Estradé, F. De la Peña <a href="mailto:Pelaezfernandezmario@gmail.com">Pelaezfernandezmario@gmail.com</a>
	9:45 – 10:00	<i>Lignin graphenization using solar concentrated energy</i> Salomé RIGOLLET, Elsa WEISS-HORTALA, Gilles FLAMANT, Ange NZIHOU <a href="mailto:salome.rigollet@mines-albi.fr">salome.rigollet@mines-albi.fr</a>
	10:00 – 10:15	<i>Supramolecular interactions between 2-dimensional Ti<sub>0.87</sub>O<sub>2</sub> functionalized with a tweezer molecule and aromatic nanomaterials</i> Ruben Canton-Vitoria, Li Longfei, Li Yan, S. Morita, S. Ando, N. Takeuchi, Eisuke Yamamoto, M. Kobayashi and Osada Minoru <a href="mailto:rcanton@imass.nagoya-u.ac.jp">rcanton@imass.nagoya-u.ac.jp</a>
Invited Speaker	10:15 – 10:50	<i>Fibres of carbon nanotube intercalation compounds and the prospect of replacing copper</i> Juan José Vilatela <a href="mailto:juanjose.vilatela@imdea.org">juanjose.vilatela@imdea.org</a>
10:50 – 11:15		COFFEE BREAK
11:15 – 13:10	Session - VIII	Chairs: J.J. Vilatela & P. Ayala
Invited Speaker	11:15-11:50	<i>Chemical modification of transition metal dichalcogenides with photoactive components</i> Nikos Tagmatarchis <a href="mailto:tagmatar@eie.gr">tagmatar@eie.gr</a>
	11:50-12:05	<i>Detailed TEM Studies of 1D nanostructures based on layered cobalt oxide</i> Raul Arenal, S. Hettler, K. Singha Roy, Leela Panchakarla <a href="mailto:arenal@unizar.es">arenal@unizar.es</a>
	12:05-12:20	<i>Structure of carbon nanotube fiber intercalation compounds with halogens and metal halides</i> Ana Inés de Isidro Gómez, A. Mikhailchan, V. Vassilev, Humberto Terrones, Javier Llorca, Johan Christensen, Juan J. Vilatela <a href="mailto:ana.isidro@imdea.org">ana.isidro@imdea.org</a>
	12:20-12:35	<i>2D material via molten salts: synthesis and applications</i> Efrat Ruse, Adi Lavi, Avia Lavi, Oren Regev <a href="mailto:oregev@bgu.ac.il">oregev@bgu.ac.il</a>
Invited Speaker	12:35-13:10	<i>One-dimensional graphene for laser physics</i> Fedotov P.V., Chizhov P.A., Obratsova E.A., Votyakov S.A., Osadchy A.V., KOZLOV A., <b>Obratsova Elena.D.*</b> <a href="mailto:elobr@mail.ru">elobr@mail.ru</a>

Thursday 16<sup>th</sup> January 2025

18:45 – 20:10	Session - IX	Chairs: W. Maser & R. Arenal
Invited Speaker	18:45-19:20	<i>Investigation of the local atomic structure and properties in 2D crystal heterostructures using STEM</i> Nasim Alem, Sai Bachu, Mathieu Kociak, Luiz HG Tizei <a href="mailto:nua10@psu.edu">nua10@psu.edu</a>
	19:20-19:35	<i>Exotic core-shell nanotubes synthesized via Van der Waals epitaxy</i> Vojtech Kundrat; Lothar Houben; Reshef Tenne <a href="mailto:vojtech.kundrat@weizmann.ac.il">vojtech.kundrat@weizmann.ac.il</a>
	19:35-19:50	<i>Vertical heterostructure of 2D-materials: from sensing to wrinkle engineering</i> M. Tripathi*, S. A. Iyengar, A.A. Graf, Rosa Garriga, Edgar Muñoz, P.M. Ajayan, A.B. Dalton <a href="mailto:mt520@sussex.ac.uk">mt520@sussex.ac.uk</a>
	19:50-20:05	<i>C60 catalysis in the prebiotic origin of life</i> Eftal Gezer, Dogan Erbahar <a href="mailto:egezer@gtu.edu.tr">egezer@gtu.edu.tr</a>
	20:05-20:10	<i>Concluding remarks</i>
21:00		<i>Congress Dinner</i>