

7th International Symposium on the Gas-phase Synthesis of Functional Nanomaterials | May 04–06, 2024

Fundamental Understanding, Modeling and Simulation, Scale-up and Application

Venue: NETZ Building, Carl-Benz-Str. 199, 47057 Duisburg
<https://www.uni-due.de/cenide/netz/en/contact.php>

Keynote presentation: up to 35 min. + at least 10 min. for discussions

Contributed presentation: up to 15 min. + at least 5 min. for discussions

| Monday, May 4 th | |
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| 12:00–13:00 | Arrival and registration |
| 13:00–13:15 | Welcome <u>Christof Schulz</u> (University of Duisburg-Essen) |
| Diagnostics and data analysis 1 (Chair: Sebastian Kaiser) | |
| 13:15–14:00 Keynote | Spectroscopy of reactive molecules: Applications to gas-phase growth species in nanoparticle synthesis <u>Josh Baraban</u> (Ben-Gurion University of the Negev) |
| 14:00–14:20 | Modeling framework for phase-selective LIBS of nanoparticles <u>Jan Menser</u> , Christof Schulz (University of Duisburg-Essen) |
| 14:20–14:40 | In situ characterization of the spectral dependence of the optical absorption function of flame-synthesized TiO₂ nanoparticles using a color digital camera and CFD simulations <u>Ipsita Choudhury</u> , Junghwa Yi, Jérôme Bonnet, Benedetta Franzelli (Paris-Saclay University) |
| 14:40–15:00 | In situ discrimination of liquid and solid iron oxide nanoparticles in plasma synthesis by absorption spectroscopy <u>Mohamed Elashry</u> ¹ , Torsten Endres ¹ , Niklas Jüngst ¹ , Guannan Liu ² , Christof Schulz ¹ (¹ University of Duisburg-Essen, ² Nanjing University of Science and Technology) |
| 15:00–15:20 | Modeling light scattering from crumpled few-layer graphene: A comparison of crumpling modeling approaches <u>Halil Ibrahim Yazici</u> ¹ , Torsten Endres ¹ , Christof Schulz ¹ , Kyle Daun ² (¹ University of Duisburg-Essen, ² University of Waterloo) |

15:20–15:45 **Coffee break**

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| Diagnostics and data analysis 2 (Chair: Torsten Endres) | |
| 15:45–16:30 Keynote | Optical diagnostics and applications of flame-synthesized nanoparticles <u>Silvana De Iuliis</u> (Italian National Research Council) |
| 16:30–16:50 | Laser-optical in situ detection of hetero-aggregate formation during gas-phase synthesis and mixing of TiO₂ and few-layer graphene <u>Felix Ebertz</u> , Philipp Leistikow, Hartmut Wiggers, Torsten Endres, Christof Schulz (University of Duisburg-Essen) |
| 16:50–17:10 | An intercomparison using the centrifugal particle Mass Analyzer-Electrometer Reference Mass Standard (CERMS) for the calibration of black carbon mass instrumentation instruments for measuring aerosol nanoparticles <u>Greg Smallwood</u> (National Research Council Canada) |
| 17:10–17:40 | Discussion: Diagnostics and data analysis |
| 17:40–18:10 | Poster short presentations All poster presenters |
| Tuesday, May 5th | |
| Fundamentals of particle formation, reaction, and growth 1 (Chair: Hartmut Wiggers) | |
| 9:00–9:45 Keynote | Hetero aggregates from the gas phase – building blocks for many applications <u>Lutz Mädler</u> (University of Bremen) |
| 9:45–10:05 | Plasma–solid reaction of methane and TiO₂ to produce hydrogen and TiC/C nanocomposite via plasma-catalytic pyrolysis <u>Jafar Fathi</u> ¹ , Maksym Buryi ¹ , Michal Hlína ¹ , Ondřej Jankovský ² , Alan Mašláni ¹ , Filip Průša ² , Vineet Sikarwar ¹ (¹ Czech Academy of Sciences, ² University of Chemistry and Technology) |
| 10:05–10:25 | Crystal defect characterization and cold plasma treatment of mesoporous CeO₂ nanoparticles synthesized via salt-assisted spray pyrolysis <u>Benedikt Eberhardt</u> ¹ , Jalal Poostforooshan ¹ , Alfred Weber ¹ , Yiannis Deligiannakis ² (¹ Clausthal University of Technology, ² University of Ioannina) |
| 10:25–10:50 | Coffee break |
| 10:50–11:10 | Theoretical study of the reaction kinetics of silene species with OH radicals <u>Qilong Fang</u> ¹ ; Jun Fang ² , Wei Li ² , Yuyang Li ² (¹ King Abdullah University of Science and Technology, ² Shanghai Jiao Tong University) |

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| 11:10–11:30 | Reactivity of graphene defect sites with molecular oxygen: Gas-phase kinetics <u>Fabiola Destro</u> ¹ , René Fournet ¹ , Pierre-Alexandre Glaude ¹ , Amitesh Jayaraman ² , Nikolaos Kateris ³ , Andrea Nobili ² , Baptiste Sirjean ¹ , Hai Wang ² (1)Université de Lorraine, (2)Stanford University, (3)University of Cambridge) |
| 11:30–11:50 | Investigating the transition between graphene and soot formation in the gas phase: A shock-tube approach <u>Ornel Padilla</u> ¹ , Kyle Daun ² , Christof Schulz ¹ , Can Shao ¹ , Hartmut Wiggers ¹ (1)University of Duisburg-Essen, (2)University of Waterloo) |

11:50–13:35 *Conference photo*
Poster session & lunch

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| Fundamentals of particle formation, reaction, and growth 2 (Chair: Christof Schulz) | |
| 13:35–14:20 Keynote | Watching materials form and transform: Structural insights into phase changes during synthesis <u>Andrea Kirsch</u> (Ruhr University Bochum) |
| 14:20–14:40 | Nanocubes and cuboctahedra: Entropic stabilization versus thermal segregation in rock salt- and spinel-type multinary oxides from spray-flame synthesis <u>Hartmut Wiggers</u> ¹ , Mohammed-Ali Sheikh ¹ , Steven Angel ¹ , Sabrina Schleich ¹ , Leon Müller ¹ , Jan Ternieden ² , Christof Schulz ¹ (1)University of Duisburg-Essen, (2)Max-Planck-Institut für Kohlenforschung) |
| 14:40–15:00 | Revealing transformation of multi-elements in flame synthesis by phase-selective laser-induced breakdown spectroscopy (PS-LIBS) <u>Yiyang Zhan</u> , Tianyi Wu, Shuting Lei, Shuiqing Li (Tsinghua University) |
| 15:00–15:20 | Particle–bath-gas interaction and matter exchange during flame synthesis: The prototypical case of iron oxide <u>Igor Rahinov</u> ¹ , Matthieu Lalanne ¹ , Piotr Cwiek ² , Yasin Karakaya ³ , Niklas Schmelzer ² , Monika Nanjiah ² , Sergey Cheskis ⁴ , Tina Kasper ³ , Christof Schulz ² , Thomas Dreier ² , Irenäus Wlokas ² (1)The Open University of Israel, (2)University of Duisburg-Essen, (3)Paderborn University, (4)Tel Aviv University) |
| 15:20–15:50 | Discussion: Fundamentals of particle formation, reaction, and growth |

15:50–16:20 *Coffee break*

| Modeling and simulation 1 (Chair: Irenäus Wlokas) | |
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| 16:20–16:40 | A thermodynamic resolution of molecular clustering: Eliminating sticking efficiency <u>Nickolas Eaves</u> (University of Windsor) |
| 16:40–17:00 | CarbonX: A process design tool for the gas-phase synthesis of metal nanoparticles and carbon nanotubes <u>Hossein Rahbar</u> , M. Reza Kholghy (Carleton University) |
| 17:00–17:20 | Rationalizing quantum-dot behavior in flame-formed carbon nanoparticles: From accurate excitation energies to stacking effects <u>Luna Pratali Maffei</u> ¹ , Andrea Nobili ² , Nikolaos Kateris ³ , Amitesh S. Jayaraman ² , Matteo Tommasini ¹ , Hai Wang ² (¹ Politecnico di Milano, ² Stanford University, ³ University of Cambridge) |
| 17:20–17:40 | Molecular dynamics simulation of carbon coating on iron-oxide nanoparticles in laminar flame synthesis <u>Maxwell Robbins</u> ¹ , Benedetta Franzelli ¹ , Eirini Goudeli ² (¹ Paris-Saclay University, ² The University of Melbourne) |

19:00–23:00 *Dinner* at Webster Brauhaus, Dellplatz 14, 47051 Duisburg

| Wednesday, May 6th | |
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| Modeling and simulation 2 (Chair: Andreas Kempf) | |
| 9:00–9:20 | A multi-modal monodisperse model for hetero-aggregate formation in aerosol streams <u>Amir Karimi Noughabi</u> , Andreas Kempf, Irenäus Wlokas (University of Duisburg-Essen) |
| 9:20–9:40 | Effects of ammonia, ethanol, and dimethyl ether (DME) blending on soot formation in ethylene combustion <u>Patrizia Crepaldi</u> , Tiziano Faravelli, Luna Pratali Maffei (Politecnico di Milano) |
| 9:40–10:10 | Discussion: Modeling and simulation |

10:10–10:35 *Coffee break*

| Scale-up and application 1 (Chair: Niklas Jüngst) | |
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| 10:35–11:20 Keynote | Plasma synthesis, surface functionalization, and emerging applications of silicon nanocrystals <u>Uwe Kortshagen</u> (University of Minnesota) |
| 11:20–11:40 | Spray-flame synthesis of doped LaMnO₃ nanoparticles for magnetocaloric applications: Toward high-throughput inline and <i>in situ</i> diagnostics <u>Shabbir Tahir</u> , Veysel Ersoy, Christof Schulz, Hartmut Wiggers (University of Duisburg-Essen) |
| 11:40–12:00 | Atomic layer deposition on particulate materials – applications in catalysis and energy <u>Ruud van Ommen</u> (Delft University of Technology) |

12:00–13:30 *Poster session & lunch*

| Scale-up and application 2 (Chair: Christof Schulz) | |
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| 13:30–13:50 | Solvent-free spray-flame synthesis based on organometallic compounds <u>Hans Orthner</u> , Evdoxia Papadimitriou, Hartmut Wiggers, Christof Schulz (University of Duisburg-Essen) |
| 13:50–14:10 | From solar panel to 3D print: Scalable microwave plasma processing of end-of-use PV silicon for laser powder bed fusion <u>Sophie Marie Schnurre</u> ¹ , Stefan Kuns ¹ , Clemens Kunz ² , Frederik Kunze ¹ , Negin Beryiani Nezafat ³ , Gabi Schierning ³ , Julia Kristin Hufenbach ² (¹ Institute of Energy and Environmental Technology ² Leibniz Institute for Solid State and Materials Research, ³ University of Duisburg-Essen) |
| 14:10–14:30 | Free-standing 2D carbon materials from plasma synthesis for energy applications <u>Hartmut Wiggers</u> ¹ , Paolo Fortugno ¹ , Claudia Francisca López-Cámara ² , Christof Schulz ¹ (¹ University of Duisburg-Essen, ² Eindhoven University of Technology) |
| 14:30–15:10 | Discussion scale-up and application |
| | Concluding remarks |
| 15:10 | Optional lab tours |

Posters

1. **Spray-flame synthesis of high-entropy catalysts for oxygen evolution reaction (OER)**
Yuanxi Li, Shuiqing Li, Yiyang Zhang
(Tsinghua University)
2. **Simultaneous imaging of PAHs, soot and OH with laser-based methods in an optical spark-ignition engine**
Esra Bauer, Sebastian Kaiser
(University of Duisburg-Essen)
3. **Decoding growth conditions: Spatial temperature mapping in carbon-rich plasma flows via NO-LIF**
Mandy Schaffeld, Christof Schulz, Hartmut Wiggers
(University of Duisburg-Essen)
4. **Novel kinetic-based sectional model for iron nanoparticles formation and growth**
Patrizia Crepaldi, Amalia Ricciardi, Tiziano Faravelli, Matteo Pelucchi
(Politecnico di Milano)
5. **Kinetics insight into hexamethyldisiloxane pyrolysis and combustion**
Qilong Fang^{1,4}, Paul Sela², Holger Somnitz², Jun Fang¹, Jürgen Herzler², Long Zhao³,
Yuyang Li¹, Christof Schulz², Mustapha Fikri²
(¹Shanghai Jiao Tong University, ²University of Duisburg-Essen,
³University of Science and Technology of China,
⁴King Abdullah University of Science and Technology)
6. **Optimizing the operating conditions of iron oxide nanoparticles synthesized by flame spray pyrolysis using SpraySyn burner**
Arona Sottas, Adam Bertrand, Marc Briant, Benedetta Franzelli, Yann Leconte, Olivier Sublemontier, Edouard de Rolland Dalon
(Paris-Saclay University)
7. **Plasma-derived Si-doped graphene as an anchoring matrix for silicon nanoparticles: Enhancing interfacial stability in Li-ion anodes**
Mohammad Amin Saadati, Hartmut Wiggers
(University of Duisburg-Essen)
8. **An overview of recent developments of the flame spray pyrolysis platform at Université Paris-Saclay**
Adam Bertrand, Marc Briant, Guilhem Dezanneau, Benedetta Franzelli, Yann Leconte, Rosario Mendez-Tovar, Remith Pongilat, Arona Sottas, Olivier Sublemontier, Said Yagoubi, Edouard de Rolland Dalon
(Paris-Saclay University)
9. **A monte carlo model for hetero-aggregate formation in aerosol streams**
Amir Karimi Noughabi, Andreas Kempf, Irenäus Wlokas
(University of Duisburg-Essen)
10. **Synthesis of Si-nanoparticles in a radio frequency plasma reactor (RF-Plasma)**
Alexander Eitner, Hartmut Wiggers
(University of Duisburg-Essen)

11. Instantaneous temperature and OH concentration imaging by two-line OH-LIF in spray-flame nanoparticle

Torsten Endres, Sadrollah Karaminejad, Thomas Dreier, Christof Schulz
(University of Duisburg-Essen)

12. 3D tomographic imaging in energy and process technology

Khadijeh Mohri, Cheau Tyan Foo
(University of Duisburg-Essen)

13. Temperature and phase evolution of individual iron and iron-oxide particles during combustion and hydrogen plasma reduction

SayedMehrdad Bathaei¹, Jonas Thiel², Marc Böke², Torsten Endres¹, Niklas Jüngst¹,
Achim von Keudell², Christof Schulz¹
(¹University of Duisburg-Essen, ²Ruhr University Bochum)