

## Program at a Glance:

Gas-phase synthesis allows the production of a large variety of complex nanoparticles for various applications and is especially suited for scaling-up, already proven by several industrial processes. In this two-day international symposium at the UDE the fundamentals of particle formation and growth in relevant nanoparticle synthesis processes such as plasma and flame synthesis are presented. Furthermore, recent model-based approaches and simulation to predict synthesis processes and particle properties are discussed. Finally, the industrial-relevant scale-up of synthesis processes and possible applications of the produced nanomaterials are presented.

This international symposium is organized within the frame of the Horizon 2020 project „Nano-materials via Gas-Phase Synthesis: A Design-Oriented Modelling and Engineering Approach“ (NanoDome) and the DFG research unit FOR 2284 „Model-based scalable gas-phase synthesis of complex nanoparticles“.



## Further Information & Contact:

**Registration (Deadline: March 12, 2017)**

<http://udue.de/synthesis2017>

### Contact

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### Venue

University of Duisburg-Essen  
NETZ – NanoEnergyTechnologyCenter  
Carl-Benz-Straße 199  
47057 Duisburg  
Germany

## Rhine-Ruhr: In the Heart of Europe



The University of Duisburg-Essen (UDE) is located in the Rhine-Ruhr metropolitan region, in the heart of Europe. With more than 11 million inhabitants, it is Germany's largest and Europe's fifth largest metropolitan region. It is named after the Rhine and Ruhr rivers, which are the region's defining geographical features and historically its economic backbone. Its location makes it well connected to other major European cities such as Amsterdam, Paris, London, Munich, Hamburg, Berlin, and Frankfurt. The region has transformed itself from a center for heavy industry into a hub for knowledge, technology, and service, and continues to have enormous economic importance. In 2010 the Rhine-Ruhr region was elected European Capital of Culture.

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UNIVERSITÄT  
DUISBURG  
ESSEN

*Offen im Denken*

**Symposium**  
**Gas-phase Synthesis of Functional Nano-**  
**materials: Fundamental Understanding,**  
**Modeling and Simulation, Scale-up**

**University of Duisburg-Essen, Germany**  
**March 21–22, 2017**

## Tuesday, March 21

12:50 Welcome by Emanuele Ghedini and Christof Schulz

### Fundamentals of Particle Formation and Growth

(Chair: Christof Schulz, University of Duisburg-Essen)

- 13:10 Gas-phase Synthesis and Characterization of Silicon-based Nanoparticles (Julia Lyubina, Evonik)
- 13:35 Mechanistic Insight into Spray-flame Synthesis: The Case of Titania (Wolfgang Peukert, University of Erlangen-Nürnberg)
- 14:00 Pushing the Sensitivity of Mass Spectrometric Detection of Nanoparticle Precursors (Tina Kasper, University of Duisburg-Essen)
- 14:25 Spectroscopic Analysis for Understanding the Growth Process of Graphene Nanoflakes in Inductively-coupled Thermal Plasma (Marc Leparoux, EMPA)
- 14:50 Settling of fumed SiO<sub>2</sub> nanoparticles and cytotoxicity (Sotiris Pratsinis, ETH Zürich)
- 15:10 **Coffee Break and Posters**
- 15:40 Rainbow Spectrometry to Determine Temperature Gradients in Droplets During Spray-flame-based Nanoparticle Synthesis (Lutz Mädler, University of Bremen)
- 16:05 Optical Band-gap Measurements for Carbonaceous Particles in Flames: Measurements and their Interpretation (Houston Miller, George Washington University, Washington DC)
- 16:30 Optical Properties of Gas-borne Silicon Nanoparticles: Optical Extinction and Laser-induced Emission (Jan Menser, University of Duisburg-Essen)
- 16:50 Mass Spectrometric Analysis of Clusters and Nanoparticles During the Gas-phase Synthesis of Tungsten Oxide (Sebastian Kluge, University of Duisburg-Essen)
- 17:10 Shock Tube Study of the Decomposition of Tetramethylsilane (Paul Sela, University of Duisburg-Essen)

17:30 Routes to Nanoparticles by Chemical Vapor Synthesis with Optimized Particle Characteristics (Markus Winterer, University of Duisburg-Essen)

19:00 **Conference Dinner at „Museum der Deutschen Binnenschifffahrt“** (Address: Apostelstraße 84, 47119 Duisburg, www.binnenschifffahrtsmuseum.de)

## Wednesday, March 22

### Modeling and Simulation

(Chair: Andreas Kempf, University of Duisburg-Essen)

- 09:00 Designing of Novel Nanomaterials (Angela Violi, University of Michigan)
- 09:25 Physico-chemical Simulation of Inorganic and Organic Nanoparticles in Combustion Devices (Amit Bhave, CMCL Innovations)
- 09:50 Reaction Kinetics and Structure of Laminar, Particle Forming Flames: Silica and Iron Oxide (Irenäus Wlokas, University of Duisburg-Essen)
- 10:10 The Nanodome Project (Emanuele Ghedini, University of Bologna)
- 10:30 **Coffee Break and Posters**
- 10:50 Modeling and Simulation of Nanopowder Growth Processes around Thermal Plasma Flows (Masaya Shigeta, Osaka University)
- 11:15 Langevin Dynamics Simulation of Nanoparticle Agglomeration in Turbulent Flows (Andreas Kronenburg, University of Stuttgart)
- 11:40 Monte Carlo-Based Population Balance Modeling in Gas-phase Synthesis (Einar Kruis, University of Duisburg-Essen)
- 12:00 Molecular Modeling of Nucleation Times, Interactions, and Sintering of Nanoparticles in Plasmas (Giovanni Barcaro and Luca Sementa, CNR Pisa)
- 12:20 Detailed Modeling of Titania and Silica Nanoparticle Precursor Chemistry (Daniel Nurkowski, Cambridge University)
- 12:40 **Lunch and Posters**

### Scale-up and Application

(Chair: Emanuele Ghedini, University of Bologna)

- 13:30 Lessons Learned from Scale-up of Flame Synthesis of Battery Cathode Material (Hai Wang, Stanford University)
- 13:55 Synthesis of Pure and Doped Ceria in a Spray Flame Reactor on the Pilot Plant Scale (Tim Hülser, IUTA, Duisburg)
- 14:15 Thermal Plasma Synthesis of Nanoparticles as Reinforcement Material for Composites with Outstanding Mechanical Properties (Marc Leparoux, EMPA)
- 14:35 Long-term Synthesis of Highly Specific Silicon Nanoparticles in a Microwave Supported Plasma Reactor on the Pilot-plant Scale (Frederik Kunze, IUTA, Duisburg)
- 14:55 Scale-up of Optical Diagnostics: From Lab-scale to Pilot-Plant Reactors (Christof Schulz, University of Duisburg-Essen)
- 15:15 Simulation of Scale-up Effects of Nanoparticle Synthesis Reactors (Andreas Kempf, University of Duisburg-Essen)
- 15:35 **Coffee Break and Posters**
- 16:00 Labtour NanoEnergyTechnologyCenter (NETZ)
- 17:00 **End**

