

5th International Symposium

Gas-Phase Synthesis of Functional Nanomaterials

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

October 11–12, 2022

Venue: Die Wolfsburg, Falkenweg 6, 45478 Mülheim an der Ruhr; www.die-wolfsburg.de/

Keynote presentation: up to 25 min. + at least 5 min. for discussions

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

Tuesday, October 11, 2022

12:45–13:15	Registration and welcome
13:15–13:30	Welcome Christof Schulz (University of Duisburg-Essen)

Fundamentals of Particle Formation and Growth (Chair: Mustapha Fikri)

13:30–14:00 Keynote	Surface reactivity and processing properties of metal oxide nanoparticles for ceramics Oliver Diwald (Paris-Lodron University Salzburg)
14:00–14:20	Influence of the carrier gas composition on the structure of metallic nanoparticles <u>A. Weber</u> , V. Olszok, P. Rembe, M. Bierwirth (TU Clausthal)
14:20–14:40	Revisiting iron oxidation chemistry in synthesis flames: insight from shock tube studies with intracavity laser absorption spectroscopy tracking of FeO <u>I. Rahinov</u> ¹ , M.R. Lalanne ¹ , P. Fjodorow ² , S. Mujaddadi ² , M. Nanjaiah ² , V.M. Baev ³ , S. Cheskis ⁴ , J. Herzler ² , M. Fikri ² , I. Wlokas ² , C. Schulz ² (¹ The Open University of Israel, ² University of Duisburg-Essen, ³ University of Hamburg, ⁴ Tel Aviv University)
14:40–15:00	Early formation of oxide nanoparticles in iron-doped flames <u>M.R. Lalanne</u> ¹ , P. Wollny ² , M. Nanjaiah ² , J. Menser ² , H. Wiggers ² , C. Schulz ² , S. Cheskis ³ , I. Wlokas ² , I. Rahinov ¹ (¹ The Open University of Israel, ² University of Duisburg-Essen, ³ Tel Aviv University)
15:00–15:20	The chemistry of siloxanes and silanols: Challenges and opportunities R.S. Tranter (Argonne National Laboratory)

15:20–15:40 **Coffee Break**

Modeling and Simulation (Chair: Irenäus Wlokas)

15:40–16:00	Atomistic insight into mechanisms of surface desorption and carbon coating on titania nanoparticles at high temperatures D. Hou ¹ , Q. Mao ² , <u>Y. Ren</u> ³ , K. Luo ¹ (¹ University College London, ² University of Duisburg-Essen, ³ RWTH Aachen University)
16:00–16:20	Role of particle liquid-phase precipitation and growth in flame spray synthesis <u>I. Skenderović</u> ¹ , A. Abdelsamie ² , S. Kuns ¹ , D. Thévenin ² , H. Wiggers ¹ , E. Kruis ¹ (¹ University of Duisburg-Essen, ² Otto von Guericke University, Magdeburg)

16:20–16:40	Crystallization dynamics of aerosol Au nanoparticles <u>Y. Wang</u> , S.E. Pratsinis (ETH Zürich)
Fundamentals of Particle Formation and Growth of Carbonaceous Materials (Chair: Hartmut Wiggers)	
16:40–17:00	Porosity and crystallinity dynamics of carbon black during internal and surface oxidation <u>G.A. Kelesidis</u> , N. Rossi, S.E. Pratsinis (ETH Zürich)
17:00–17:20	Ultra-fine graphite nanoparticles formed in high-temperature premixed flames <u>J. Camacho</u> (San Diego State University)
17:20–17:40	Morphology evolution of plasma-synthesized few-layer graphene <u>C.-F. Lopez-Camara</u> , P. Fortugno, H. Wiggers (University of Duisburg-Essen)
17:40–18:00	Partitioning of Pd on the surface and into the bulk of FSP-made Pd-containing SnO ₂ and its impact on CO & acetone sensing <u>K. Jabłczyńska</u> ^{1,2} , S.E. Pratsinis ¹ (¹ ETH Zürich, ² Warsaw University of Technology)
18:00–19:00	Dinner at the conference venue
19:00–21:00	Poster session

Wednesday, October 12, 2022

8:00–9:00 **Breakfast**

Diagnostics and Data Analysis (Chair: Seung-Jin Baik)

9:00–9:30 Keynote	Monitoring and control of flame spray pyrolysis via artificial intelligence Noah H. Paulson (Argonne National Laboratory)
9:30–9:50	Autonomous measurements of laminar flame speed in particle forming flames <u>J. Menser</u> , F. Ebertz, T. Endres, C. Schulz, I. Wlokas (University of Duisburg-Essen)
9:50–10:10	Visualization and statistical analysis of droplet puffing and micro-explosion in spray-flame synthesis <u>N. Jüngst</u> ¹ , G.J. Smallwood ² , S.A. Kaiser ¹ (¹ University of Duisburg-Essen, ² National Research Council Canada)

10:10–10:30 **Coffee break**

Diagnostics and Data Analysis (Chair: Torsten Endres)

10:30–11:00 Keynote	Characterization of functionalized particles in gases and liquids by X-ray scattering methods <u>Hermann Nirschl</u> , J. Ungerer, S. Buchheiser (Karlsruhe Institute of Technology (KIT))
11:00–11:20	Tomographic imaging using multi-simultaneous measurements (TIMes) for emission reconstructions in the context of nanoparticle synthesis in SpraySyn flames <u>F.J.W.A. Martins</u> , C.T. Foo, A. Unterberger, K. Mohri (University of Duisburg-Essen)
11:20–11:40	Scale-up: spray-flame synthesis of nanoparticles on a pilot scale <u>M. Underberg</u> ¹ , M. Prenting ² , M. Sieber ³ , T. Hülser ¹ , S.M. Schnurre ¹ (¹ Institut für Energie- und Umwelttechnik e.V. (IUTA), ² University of Duisburg-Essen, ³ Technische Universität Berlin)

11:40–12:05	SpraySyn: a flame simulation comparison <u>A. Kempf</u> , S.-J. Baik (University of Duisburg-Essen)
12:05–13:00	Lunch

Scale-up and Application (Chair: Tim Hülser)	
13:00–13:20	Nanoscale high-entropy oxides (HEO) from spray-flame synthesis for oxygen evolution reaction (OER) in water splitting and catalytic cyclohexene oxidation <u>S. Angel</u> ¹ , V. Chanda ¹ , I. Sanjuán Moltó ¹ , J. Büker ² , C. Andronesco ¹ , M. Muhler ² , C. Schulz ¹ , H. Wiggers ¹ (¹ University of Duisburg-Essen, ² Ruhr-University Bochum)
13:20–13:40	Flame-Made Quantum Dots <u>K.B. Riad</u> ¹ , J. Peters ¹ , M.R. Kholghy ¹ , P.M. Wood-Adams ² (¹ Carleton University, Ottawa, ² Concordia University, Montreal)
13:40–14:00	Recent advances in combustion aerosol-made gas sensors <u>A.T. Güntner</u> ^{1,2} , I.C. Weber ¹ , S.E. Pratsinis ¹ (¹ ETH Zürich, ² University Hospital Zürich)

14:00–14:20 **Coffee break**

Modeling and Simulation (Chair: Einar Kruis)	
14:20–14:40	Numerical simulations of TiO ₂ nanoparticle synthesis in sooting and non-sooting laboratory-scale flames <u>Y. Ogata</u> ¹ , J. Yi ¹ , A. Cuoci ² , C. Betrancourt ¹ , B. Franzelli ¹ (¹ EM2C Laboratory, Université Paris-Saclay, CNRS, ² Politecnico di Milano)
14:40–15:00	Numerical investigation of laminar methane flames doped with iron(III) nitrate/butanol aerosol in a novel matrix burner <u>M. Nanjaiah</u> ¹ , P. Wollny ¹ , S. Apazeller ¹ , M. Gonchikzhapov ² , P. Narasu ³ , E. Gutheil ³ , H. Wiggers ¹ , C. Schulz ¹ , T. Kasper ² , A. Kempf ¹ , I. Wlokas ¹ (¹ University of Duisburg-Essen, ² University of Paderborn, ³ University of Heidelberg)
15:00–15:20	Sintering rate of nickel nanoparticles by molecular dynamics <u>H. Rahbar</u> ¹ , E. Goudeli ² , M.R. Kholghy ¹ (¹ Carleton University, Ottawa, ² University of Melbourne)
15:20–15:50 Keynote	Imaging molecular real - Examining non-equilibrium processes at the molecular relaxation processes in complex fluids environments Matthias Ihme (Stanford University)

15:50–16:00 **Concluding remarks**
Christof Schulz (University of Duisburg-Essen)

Poster

1. A new dual matrix burner for one-dimensional investigation of aerosol flames
S. Apazeller¹, M. Gonchikzhapov², M. Nanjaiah¹, T. Kasper², I. Wlokas¹, H. Wiggers¹, C. Schulz¹ (¹ University of Duisburg-Essen, ² University of Paderborn)
2. Large-eddy simulations of nanoparticle synthesis in spray flames
S.-J. Baik, P. Wollny, M. Nanjaiah, I. Wlokas, A. Kempf (University of Duisburg-Essen)

3. Direct numerical simulations of turbulent premixed and non-premixed methane/air particle-forming flames
L. Cifuentes, I. Wlokas, A. Kempf (University of Duisburg-Essen)
4. Rapid and selective NH₃ sensing by porous CuBr
M. D'Andria, M. Wied, N. J. Pineau, S. E. Pratsinis, A. T. Güntner (ETH Zürich)
5. Handheld device for selective benzene sensing over toluene and xylene
S. Hersberger, M. D'Andria, I. C. Weber, P. Rüedi, P. Šot, S. E. Pratsinis, A. T. Güntner (ETH Zürich)
6. A burner arrangement for nanoparticle flame synthesis under pulsed conditions as a platform to study the influence of turbulence
A. El Moussawi, T. Endres (University of Duisburg-Essen)
7. Laser-optical in situ detection and imaging of gas-borne hetero aggregate formation
L. Engelbracht-Kloß, F. Ebertz (University of Duisburg-Essen)
8. Measurements of gas-phase iron species using advanced laser-spectroscopy tools
P. Fjodorow¹, M. R. Lalanne², M. Fikri¹, J. Herzler¹, M. P. Frolov³, S. O. Leonov³, V. I. Kozlovsky³, I. Rahinov², C. Schulz¹ (¹ University of Duisburg-Essen, ² The Open University of Israel, ³ Lebedev Physical Institute of the Russian Academy of Sciences)
9. Gas phase synthesis of functional silicon/carbon hetero aggregates
P. Fortugno, H. Wiggers (University of Duisburg-Essen)
10. Insights into the gas-phase synthesis of silica nanoparticles in HMDSO-doped flames
Y. Karakaya and Tina Kasper (University of Paderborn)
11. Investigation of spray parameters and flame stability in two modified nozzle configurations of the SpraySyn burner
S. Karaminejad¹, S. M.L. Dupont², M. Bieber², M. A. Reddemann², R. Kneer², T. Dreier¹, T. Endres¹, C. Schulz¹ (¹ University of Duisburg-Essen, ² RWTH Aachen University)
12. An enhanced joint Eulerian-Lagrangian method for the multiscale simulation of aerosol mixing at high Schmidt numbers
A. Karimi Noughabi, I. Wlokas, A. Kempf (University of Duisburg-Essen)
13. Spatially resolved measurement of the distribution of solid and liquid Si nanoparticles in plasma synthesis through line-of-sight extinction spectroscopy
G. Liu¹, P. Wollny¹, J Menser¹, Thomas Dreier¹, Torsten Endres¹, Irenaeus Wlokas¹, Kyle J. Daun², Christof Schulz¹ (¹ University of Duisburg-Essen, ² University of Waterloo, Canada)
14. Temperature dependent properties and sintering kinetics of Iron nanoparticles
Q. Mao, I. Skenderović, F. E. Kruis (University of Duisburg-Essen)
15. Liquid-phase temperature in the SpraySyn flame measured by two-color laser-induced fluorescence thermometry and simulated by LES
M. M. Prenting, S.-J. Baik, T. Dreier, T. Endres, A. Kempf, C. Schulz (University of Duisburg-Essen)
16. Doped NaSICON-type solid electrolytes for sodium-Ion batteries from scalable spray-flame synthesis
M.A. Sheikh¹, L. Müller¹, P. Odenwald², H. Wiggers¹ (¹ University of Duisburg-Essen, ² Forschungszentrum Jülich))
17. A theoretical study of the energetics and kinetics of the bimolecular reaction of hexamethyldisiloxane (HMDSO) with single oxygen (³P) radicals in the gas phase synthesis of silicane nanoparticles
A. Hermsen, H. Somnitz (University of Duisburg-Essen)
18. Influence of spray flow field and Reynolds number on microexplosions in FSP
M. Stodt, J. Kiefer, U. Fritsching (University of Bremen)
19. Investigation of microexplosions and flames of burning FSP-droplets in a variably heated oxygen atmosphere
A. Witte, L. Mädler (University of Bremen)