

Program

Artificial Intelligence, Machine Learning and Data Science in Energetic Materials Research

54th International Annual Conference of the Fraunhofer ICT

combined with

Symposium "Advances in Metal Fuels and Reactive Materials Science and Technology"

June 24-27, 2025 Convention Center, Gartenhalle Karlsruhe, Germany

Introduction

The Fraunhofer ICT International Annual Conference serves as a forum to discuss the current state of the art, to present new methods, ideas, and research results and to further improve scientific understanding in the field of energetic materials. Join our conference to benefit from a platform for lively discussions, detailed exchange of scientific results and – most importantly – for networking with international experts.

Up to this day, even after decades of research and progress, the development of new energetic materials and systems still relies heavily on cost- and time-consuming trial and error. The reason for this is that the characteristics of energetic materials, such as performance, sensitivity or aging, often exhibit unexpected and very sensitive dependencies on changing environmental conditions like temperature, pressure, or chemical composition. Also, the identification of essential input parameters for established numerical simulations is often constrained by challenging experimental conditions or financial and temporal limitations which restrict the detailed characterization to only a few selected candidate materials.

New methods in the fields of artificial intelligence, machine learning and data science could revolutionize the development of new energetic materials and systems in the future. This would enable scientists to screen larger chemical spaces and a wider range of life-cycle conditions and applications than ever before, to learn about cause-effect relationships and to extract more information from datasets. However, there is a caveat. One of the main challenges is the often limited size and quality of datasets, which hinders the development of precise models and the ability to discriminate between real information and statistical noise.



The 54th International Annual Conference of Fraunhofer ICT gives energetic materials researchers a unique opportunity to discuss new methods and trends, to meet old and new colleagues and to contribute to a lively discussion. In particular, the conference offers a unique platform for young scientists and early-career researchers to present their research and to build their international network of experts.

The integration of "Advances in metal fuels and reactive materials science and technology" – a symposium organized by Dr. Carole Rossi (Toulouse/F), Dylan J. Kline (Livermore, CA/USA), Conrad J. M. Hessels (Eindhoven/NL) and Peter Schaaf (Ilmenau/D) – into the 2025 Fraunhofer ICT International Annual Conference will contribute further to its wide spectrum of scientific contributions.

Chairman of the Conference

Dr. Sebastian Wurster

Spokesman for Explosives Technology, Safety and Security Fraunhofer ICT, Pfinztal, Germany

General Information

Registration

- Register online: www.ict.fraunhofer.de/annualConference
- Registration fee (incl. proceedings, coffee breaks, lunch):€ 950,--
- Participation cannot be guaranteed for registrations arriving after June 16th, 2025. The fee has to be paid **upon receipt of** the invoice by bank transfer.

Cancellation Policy

■ € 500,-- will be charged for cancellations after June 17th, 2025.
No-shows will be charged the whole fee.

Accommodation

Online, see www.ict.fraunhofer.de/annualConference

Conference Office

- Foyer of the GARTENHALLE
- Open from Tuesday, June 24, 16.00 h till Friday, June 27, 14.00 h during the Conference and may be reached by Phone +49-(0)7 21 / 37 20 6000

Check in / Welcome Reception

- Please check in at the Conference Office on Tuesday, June 24, between 16.00 and 20.00 h.
- All participants are cordially invited to the Welcome Reception on the same day, starting at 18.00 h in the foyer of the GARTENHALLE.

Conference Language

English

Get-together (Thursday, June 26)

- The Fraunhofer ICT can be visited on Thursday, June 26 in the evening. There will be a Get-together Party with draught beer, barbecue and fireworks (after sunset). Please mark on your registration form whether you wish to participate.
- Transportation: Bus shuttle Convention Centre Karlsruhe –
 Fraunhofer ICT and back

Chairman

Dr. Sebastian Wurster (Fraunhofer ICT)

Program Committee

- Richard Gee (Lawrence Livermore National Laboratory, USA)
- Thomas M. Klapötke (LMU München, D)
- Dylan J. Kline (Lawrence Livermore National Laboratory, USA)
- Ernst-Christian Koch (Lutradyn, D)
- Henric Oestmark (FOI, SE)
- Jiri Pachman (University of Pardubice, CZ)
- Carole Rossi (LAAS-CNRS, F)

Exhibiting companies

- Prototypa-ZM, s.r.o., Brno, CZ
- Teledyne GmbH, Heidelberg, D

How to find the venue

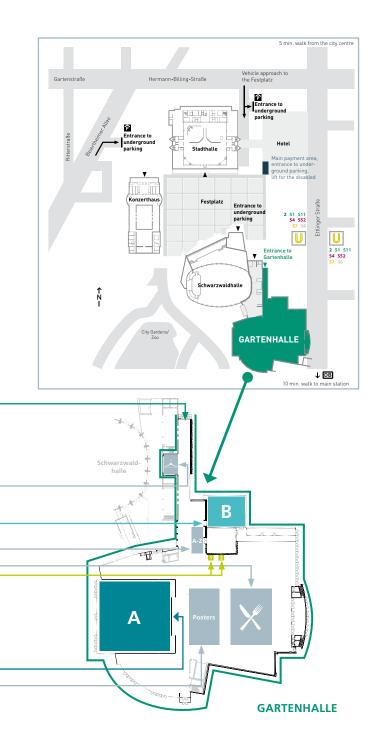
Karlsruhe is located 120 km south of Frankfurt (Main)/Frankfurt International Airport just beside the Autobahn A5, and is also connected to Frankfurt via the Intercity Express Train ICE. Additional airports are: Strasbourg (F) (approx. 100 km) and Stuttgart (D) (approx. 90 km).

By car: Coming from the A5/A8, please take exit no. 45 "Karls-ruhe-Mitte" in the direction of Karlsruhe. Leave the B10 in the direction of "Stadtmitte/Zentrum". Coming from the A 65/ or B10, please take exit no. 2 in the direction of "Kongresszentrum". Follow the signs for "Kongresszentrum".

Address:

Congress Center Karlsruhe, Festplatz 9, 76137 Karlsruhe, Germany

| Entrance to | Gartenhalle | |
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| | Wardrobe | |
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| Lecture Ro | om B | |
| | Pagistration | |
| | Registration | |
| Lunch | | |
| | Exhibitors: | |
| | 1 – Prototypa-ZM, s.r.o. | |
| | 2 – Teledyne GmbH | |
| | | |
| Lecture Ro | om A | |
| | | |
| | Posters / Poster Session | |



Tuesday, June 24

| 16.00-20.00 | Check-in |
|-------------|-------------------|
| 18.00-20.30 | Welcome Reception |

Wednesday, June 25

LECTURE ROOM A

09.00 WELCOME AND OPENING

S. Wurster

Fraunhofer ICT, Pfinztal, D

S. Wilker

BAAINBw, Koblenz, D

KEYNOTE-SESSION I

Chair: S. Wurster, Fraunhofer ICT

09.20 A1 KEYNOTE I – FEAST OR FAMINE?

AN EXPERIMENTALISTS VIEW OF ARTIFICIAL INTELLIGENCE TO ENERGETICS RESEARCH

A. Mueller

Los Alamos National Laboratory, USA

09.50 A2 KEYNOTE II – PROGRESS IN INTERTWINING ARTIFICIAL INTELLIGENCE WITH HIGH FIDELITY

MODELING TO ENHANCE MULTI-SCALE,
MULTI-PHYSICS SIMULATIONS

H. S. Udaykumar

University of Iowa, USA

10.20 **Coffee break**

Lecture Program

| | LECTURE ROOM B |
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SESSION A1

TOWARDS AN UNDERSTANDING OF SENSITIVITY OF ENERGETIC MATERIALS USING AI/ML

Chair: W. de Klerk, TNO, NL

11.00 A3 UTILIZING LARGE DATASETS OF EXPLOSIVES TO INTERPRET HANDLING SENSITIVITY TRENDS

V. W. Manner, M. J. Cawkwell, J. V. Davis, F. W. Marrs, N. Lease Los Alamos National Laboratory, USA

11.20 A4 PREDICTING DROP-WEIGHT IMPACT SENSITIVITY DIRECTLY FROM MOLECULAR STRUCTURE USING PHYSICS-INFORMED MACHINE LEARNING

E. C. Thompson, G. Hutchings, F. W. Marrs Los Alamos National Laboratory, USA

11.40 A5 MISCONCEPTIONS AND OPEN ISSUES IN ENERGETIC MATERIALS

D. Mathieu CEA DAM, Monts, F

12.00 A6 AN IMPROVED STATISTICAL ANALYSIS OF 80 SENSITIVITY DATASETS

D. Christensen, G. P. Novik FFI, NO A. van der Heijden TNO. NL

12.20 A7 PREDICTING THE SENSITIVITY OF ENERGETIC COMPOUNDS THROUGH MACHINE LEARNING: FOR DISCOVERING INSENSITIVE ENERGETIC MATERIALS

Yu-Cong Chen, Wenbin Yi School of Chemical Engineering NJUST, Nanjing, PRC

SESSION B1

PROCESSING OF BI-FUELS AND ADVANCED REACTIVE MATERIALS FOR ENHANCED PERFORMANCE

Chair: A. Esteve, LAAS-CNRS University of Toulouse, F

B1 TUNING AND AUTOMATED CHARACTERIZATION OF NANOSTRUCTURAL METAL COMPOSITES FOR COMBUSTION APPLICATIONS

K.-L. A. Chintersingh
New Jersey Institute of Technology, USA

B2 SYNTHESIS OF COLLOID ENERGETIC PARTICLES AND THEIR UNDERWATER COMBUSTION BEHAVIORS

J. Z. Wen University of Waterloo, CAN

B3 COMBUSTION CHARACTERISTICS OF FE/CUO PYROTECHNIC COMPOSITIONS

N. Mokrani, S. Bernard, L. Courty Universite Orleans, Bourges Cedex, F

B4 TITANIUM-BASED NANOTHERMITES AND NSTEXS

T. Jarosz, A. Stolarczyk Silesian University of Technology, Gliwice, PL M. Polis, K. Szydlo Institute of Industrial Organic Chemistry, Krupski Mlyn, PL

B5 TWO-DIMENSIONAL ENGINEERING OF METASTABLE INTERMOLECULAR COMPOSITES: SYNERGISTIC ENHANCEMENT OF MECHANICAL STRENGTH AND STIMULUS-SPECIFIC SENSITIVITY

Jingwei Li, Xuwen Liu

Jianghan University, Wuhan / Nanjing University of Science and Technology, Nanjing, PRC

Yaqing Cao

Nanjing University of Science and Technology, PRC Guangyu Yin, Zhangbo Ming, Zhichao Zhao, Yihao Shen Jianghan University, Wuhan, PRC

SESSION A2

MODELING AND SIMULATION OF TRANSIENT ENERGETIC MATERIAL BEHAVIOR WITH AI/ML METHODS

Chair: S. Deng, MIT, USA

14.00 A8 BAYESIAN PARAMETRIC LATENT DYNAMICS MODELING OF SHOCK-INDUCED PORE COLLAPSE PROCESS

S. W. Chung, Y. Choi, P. Tranquilli, C. M. Miller, H. Keo Springer, K. Sullivan Lawrence Livermore National Laboratory. USA

14.20 A9 EMULATING ADAPTATIVE MESH REFINEMENT FOR ENERGETIC MATERIALS WITH DEFORMABLE PHYSICS AWARE RECURRENT CONVOLUTIONAL NETWORKS (D-PARC)

J. T. Beerman, S. S. Baek University of Virginia, Charlottesville, USA P. K. Seshadri, Y.-T. Nguyen, H. S. Udaykumar University of Iowa, Iowa City, USA

14.40 A10 REDUCED ORDER MODELING OF DYNAMICAL SYSTEMS OF ENERGETIC MATERIALS USING PHYSICS-AWARE CONVOLUTIONAL NEURAL NETWORKS IN A LATENT SPACE (LatentPARC)

Z. J. Gray, S. Azarfar, S. S. Baek University of Virginia, Charlottesville, USA H. S. Udaykumar University of Iowa, Iowa City, USA

15.00 A11 A PHYSICS-AWARE DEEP LEARNING MODEL FOR SHEAR BAND FORMATION IN WEAK SHOCK REGIME

X. Cheng, B. Chen, J. Choi, S. Baek University of Virginia, Charlottesville, USA Y.T. Nguyen, P. Seshadri, M. Verma, H.S. Udaykumar University of Iowa, Iowa City, USA

15.20 **Coffee break**

SESSION B2

IN-SITU CHARACTERIZATION OF REACTION KINETICS

Chair: M. Abere, Sandia National Laboratories, Albuquerque, USA

B6 WHAT ATOMIC PROPERTIES OF METAL OXIDE CONTROL THE INITIATION TEMPERATURE WITH METAL FUELS

X. Wang

University of California, Irvine, USA

CHARACTERIZATION OF ULTRAFAST **B7 DECOMPOSITION DYNAMICS IN NITRATE** ESTER ENERGETIC MATERIALS

E. Britt, H. Lopez Pena, M. Minvielle, K. Moore Tibbetts Virginia Commonwealth University, Richmond, USA

B8 UNDERSTANDING AND CONTROLLING REACTIVITY IN THERMITES

K. T. Sullivan

Lawrence Livermore National Laboratory, Livermore, USA

OUANTIFYING THE EFFECTS OF ARTIFICIAL AGING ON B9 THE IGNITION AND REACTION OF NI/AL MULTILAYERS

D. P. Adams, S. McPherson, H. Choi, P. G. Kotula, A. Jarzembski, K. Potter, P. E. Specht, M. J. Abere Sandia National Laboratories, Albuquerque, USA G. B. Kennedy, N. N. Thadani Georgia Institute of Technology, Atlanta, USA

SESSION A3

AI/ML – STRUCTURE, PROPERTY, PERFORMANCE RELATIONS AND MOLECULAR DESIGN PREDICTIONS I

Chair: E.C. Koch, Lutradyn, D

16.00 A12 IMPROVING THE ESTIMATION OF ENTHALPIES OF FORMATION OF ENERGETIC SALTS

E. Ott, J. Glorian ISL, Saint Louis, F D. Mathieu

CEA DAM, Monts, F

16.20 A13 MACHINE LEARNING/ARTIFICIAL INTELLIGENCE BASED ENERGETIC MOLECULE DESIGN STRATEGY

Wen Qian, Jian Liu, Chaoyang Zhang Institute of Chemical Materials CAEP, Mianyang, PRC

16.40 A14 PREDICTING MOLECULAR PROPERTIES VIA INTERPRETABLE MACHINE LEARNING AND HIGH-THROUGHPUT COMPUTATIONS

M. C. Davis, J. N. Schroeder, R. Seaton Ullberg, W. Kort-Kamp, C. J. Snyder, I. Matanovic Los Alamos National Laboratory, USA

17.00 A15 SWITCH ON AMINE SUBSTRATE REACTIVITY TOWARDS HEXAAZAISOWURTZITANE CAGE: INSIGHTS FROM A TAILORED MACHINE LEARNING MODEL

Lei Zhang, Chunlin He, Kaile Dou, Siping Pang Beijing Institute of Technology, Beijing, PRC

17.20 A16 DATA- AND MECHANISM-DRIVEN EXPLAINABLE DEEP LEARNING RESEARCH ON ENERGETIC MATERIALS

Xin Huang

Institute of Chemical Materials CAEP, Mianyang, PRC

SESSION B3

IN-OPERANDO CHARACTERIZATION OF SELF-PROPAGATING REACTION

Chair: X. Mi, Eindhoven University of Technology, NL

B10 ENGINEERING MICROSCALE AGGLOMERATION AND MACROSCALE REACTION PROPAGATION OF HIGH NANO-ALUMINUM LOADING ENERGETIC COMPOSITES

H. Wang

Beijing University, Beijing, PRC

M. R. Zachariah

University of California, Riverside, USA

B11 tba

B12 INVESTIGATING THE COMBUSTION MECHANISMS OF TIB2 INTEGRATED AL/CUO NANOTHERMITES THROUGH IN-OPERANDO FLAME CHARACTERIZATION

V. Singh, A. Esteve, C. Rossi LAAS-CNRS, University of Toulouse, F

B13 EXTRACTING AND VALIDATING MECHANISMS FROM 3D SIMULATIONS OF SPIN-LIKE FLAMES IN CO/AL

M. J. Abere, D. E. Kittell, C. Sobczak, D. P. Adams Sandia National Laboratories, Albuquerque, USA R. V. Reeves

Lawrence Livermore National Laboratory, USA

B14 COMBUSTION OF LITHIUM AND MAGNESIUM FOR HEAT AND POWER GENERATION IN SPACE MISSIONS

S. Cordova, K. Estala-Rodriguez, E. Shafirovich The University of Texas, El Paso, USA

Thursday, June 26

LECTURE ROOM A

KEYNOTE SESSION II

Chair: S. Wurster, Fraunhofer ICT

09.00 A17 KEYNOTE III – MODEL CALIBRATION AND UNCERTAINTY QUANTIFICATION FOR REACTIVE MATERIALS

S. Dena

Massachussets Institute of Technology, USA

09.30 A18 KEYNOTE IV – COMBINING MACHINE LEARNING AND PHYSICS: PREDICTIVE MODELS FOR PROCESSING, INITIATION, AND PERFORMANCE OF ENERGETICS

A. Strachan

Purdue University, USA

10.00 Coffee break

SESSION A4

AI/ML- STRUCTURE, PROPERTY, PERFORMANCE RELATIONS AND MOLECULAR DESIGN II

Chair: S. Wilker, BAAINBw, D

10:40 A19 OPTIMISATION OF BATCH MIXING USING MACHINE CALCULATIONS SOFTWARE

L. Esperi, E. Tunestal

Eurenco Bofors AB, Karlskoga, SE

11.00 A20 A RAPID COMPOSITE EXPLOSIVE FORMULATION METHOD INTEGRATING MULTI-OBJECTIVE OPTIMIZATION AND MACHINE LEARNING FOR DIVERSE APPLICATIONS

Lijuan Peng, Yuxin Huang, Wenhua Zhu

Southwest University of Science and Technology,

Mianyang, PRC

Donglei Wang, Xuwang Liu, Hengjian Huang Institute of Chemical Materials CAEP, Mianyang, PRC

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| | ON B4 ERICAL MODELING FOR ANALYZING REACTION |
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| NUM MECI OF RI | ERICAL MODELING FOR ANALYZING REACTION HANISMS AND OPTIMIZING THE PERFORMANCE |
| NUM MECI OF RI Chair | ERICAL MODELING FOR ANALYZING REACTION HANISMS AND OPTIMIZING THE PERFORMANCE EACTIVE MATERIALS : J. Wen, University of Waterloo, CAN |
| NUM MECI OF RI | ERICAL MODELING FOR ANALYZING REACTION HANISMS AND OPTIMIZING THE PERFORMANCE EACTIVE MATERIALS : J. Wen, University of Waterloo, CAN MESOSCALE MODELLING OF SHOCK INDUCED |
| NUM MECI OF RI Chair | ERICAL MODELING FOR ANALYZING REACTION HANISMS AND OPTIMIZING THE PERFORMANCE EACTIVE MATERIALS : J. Wen, University of Waterloo, CAN |
| NUM MECI OF RI Chair | ERICAL MODELING FOR ANALYZING REACTION HANISMS AND OPTIMIZING THE PERFORMANCE EACTIVE MATERIALS : J. Wen, University of Waterloo, CAN MESOSCALE MODELLING OF SHOCK INDUCED REACTIONS IN NI+AL MULITLAYER THIN FILMS D. E. Kittell, P. E. Specht, M. J. Abere, K. M. Potter, |
| NUM MECI OF RI Chair | ERICAL MODELING FOR ANALYZING REACTION HANISMS AND OPTIMIZING THE PERFORMANCE EACTIVE MATERIALS : J. Wen, University of Waterloo, CAN MESOSCALE MODELLING OF SHOCK INDUCED REACTIONS IN NI+AL MULITLAYER THIN FILMS |
| NUM MECI OF RI Chair B15 | ERICAL MODELING FOR ANALYZING REACTION HANISMS AND OPTIMIZING THE PERFORMANCE EACTIVE MATERIALS : J. Wen, University of Waterloo, CAN MESOSCALE MODELLING OF SHOCK INDUCED REACTIONS IN NI+AL MULITLAYER THIN FILMS D. E. Kittell, P. E. Specht, M. J. Abere, K. M. Potter, S. L. McPherson, D. P. Adams Sandia National Laboratories, Albuquerque, USA |
| NUM MECI OF RI Chair | ERICAL MODELING FOR ANALYZING REACTION HANISMS AND OPTIMIZING THE PERFORMANCE EACTIVE MATERIALS : J. Wen, University of Waterloo, CAN MESOSCALE MODELLING OF SHOCK INDUCED REACTIONS IN NI+AL MULITLAYER THIN FILMS D. E. Kittell, P. E. Specht, M. J. Abere, K. M. Potter, S. L. McPherson, D. P. Adams Sandia National Laboratories, Albuquerque, USA DEVELOPING DIFFERENTIABLE PHASE TRANSITION |
| NUM MECI OF RI Chair B15 | ERICAL MODELING FOR ANALYZING REACTION HANISMS AND OPTIMIZING THE PERFORMANCE EACTIVE MATERIALS : J. Wen, University of Waterloo, CAN MESOSCALE MODELLING OF SHOCK INDUCED REACTIONS IN NI+AL MULITLAYER THIN FILMS D. E. Kittell, P. E. Specht, M. J. Abere, K. M. Potter, S. L. McPherson, D. P. Adams Sandia National Laboratories, Albuquerque, USA DEVELOPING DIFFERENTIABLE PHASE TRANSITION MODELS IN REACTIVE MATERIALS |
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| NUM MECI OF RI Chair | ERICAL MODELING FOR ANALYZING REACTION HANISMS AND OPTIMIZING THE PERFORMANCE EACTIVE MATERIALS : J. Wen, University of Waterloo, CAN MESOSCALE MODELLING OF SHOCK INDUCED REACTIONS IN NI+AL MULITLAYER THIN FILMS D. E. Kittell, P. E. Specht, M. J. Abere, K. M. Potter, S. L. McPherson, D. P. Adams Sandia National Laboratories, Albuquerque, USA DEVELOPING DIFFERENTIABLE PHASE TRANSITION MODELS IN REACTIVE MATERIALS |

| | LECT | URE ROOM A |
|-------|------------------------|---|
| 11.20 | A21 | DEVELOPMENT OF A ML-DRIVEN SELF-OPTIMIZATION WORKFLOW FOR THE PRODUCTION OF NITROGEN-RICH COMPOUNDS IN CONTINUOUS PROCESSING G. Araya Vargas, D. Boskovic, M. Schwarzer, A. Mendl Fraunhofer ICT, Pfinztal, D |
| 11.40 | A22 | ACCELERATING MOLECULE DISCOVERY THROUGH INVERSE DESIGN C. J. Snyder, I. Matanovic, W. Kort-Kamp, J. V. Davis, C. Garcia Cardona, M.C. Davis, A. Salij, R. Seaton Ullberg, J. N. Schroeder, L. Stevens Ouellet, L. V. Hooker, M. J. Cawkwell, R. Perriot, M. E. Hamilton, D. E. Chavez, E. S. Rivera, P. M. Mach Los Alamos National Laboratory, Los Alamos, USA |
| 12.00 | A23 | ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING FOR ENERGETICS: THE PROMISE AND THE PITFALLS R. M. Doherty Energetics Technology Center, USA |
| 12.20 | Lunc | h break |
| , | POST | TER SESSION |
| 14.00 | Poster Session (Foyer) | |
| 14.20 | Poste | r Session (Foyer) |
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B17 ATOMIC SCALE MODELLING OF GAS/SURFACE AND SOLID/SOLID INTERFACIAL CHEMISTRY IN THE REACTION OF AL/CUO THERMITE

A. Esteve, H. Jabraoui, C. Rossi LAAS University of Toulouse, CNRS, F

B18 MODELLING OF PYROTECHNIC MIXTURES

S. Knapp Fraunhofer ICT, Pfinztal, D

B19 EXPERIMENTS AND MODELING OF THERMITE REACTIONS

M. J. S. de Lemos Instituto Tecnologico de Aeronautica (ITA), Sao Jose do Campos, BR

Session B5

METAL COMBUSTION FOR SUSTAINABLE ENERGY APPLICATION (TERRESTRIAN AND SPACE APPLICATIONS) I

Chair: H. Wang, Beijing University, Beijing, PRC

B20 ON THE COMBUSTION OF FE-AL AND FE-SI POWDERS FOR SUSTAINABLE ENERGY STORAGE

L. Ahmad, Z. Bruyr, F. Contino, P. J. Jacques, L. Choisez Universite Catholique de Louvain, B Y. Li, A. Sperling, B. Böhm, A. Dreizler Technical University of Darmstadt. D

B21 ENHANCING IRON-POWDER COMBUSTOR PERFORMANCE THROUGH FUNDAMENTAL INSIGHTS

X. Mi, W. Tian, S. Hemamalini, L. Thijs, K. Zhang, N. van den Hout, Y. Shoshin, V. Kornilov, G. Finotello, B. Cuenot, P. de Goey Eindhoven University of Technology, Eindhoven, NL

| | LECT | URE ROOM A |
|-------|-------|---|
| 14.40 | Poste | r Session (Foyer) |
| 15.00 | Poste | r Session (Foyer) |
| 15.20 | Coffe | ee break |
| | RELA | on A5 L – STRUCTURE, PROPERTY, PERFORMANCE TIONS AND MOLECULAR DESIGN PREDICTIONS III : M. Heil, Fraunhofer ICT |
| 16.00 | A24 | BUILDING ENERGETIC CHEMICAL SPACES C. Wespiser, D. Mathieu, M. Daniel, E. Pasquinet CEA-DAM Le Ripault, Monts, F |
| 16.20 | A25 | MODELING THE INITIATION OF THERMO- MECHANICS OF ENERGETIC MATERIALS WITH LEARNABLE ACTIVATION FUNCTIONS J. B. Choi, Y. Cheng, S. Azarfar, C. Williams, S. Baek University of Virginia, Charlottesville, USA Y. T. Nguyen, P. Seshadri, H. S. Udaykumar University of Iowa, Iowa City, USA |
| 17.30 | | Departure from Conference Hall Bunhofer ICT |
| 18.00 | | ogether que Party, offering wine, draught beer |
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B22 DIRECT NUMERICAL SIMULATION OF AN ALUMINUM PARTICLE COMBUSTION IN OXIDIZING FLOW, WITH GAS AND CONDENSED-PHASE REACTIONS

L. Pillemont, A. Esteve, C. Rossi LAAS-CNRS, University of Toulouse, F B. Bedat, O. Simonin IMFT, University of Toulouse, F

B23 IRON AS CARBON-FREE ENERGY CARRIER IN A CIRCULAR ENERGY ECONOMY: CYCLING AT MILD CONDITIONS

A. Knapp, F. Straub, C. Kuhn, O. Deutschmann Karlsruhe Institute of Technology KIT, Karlsruhe, D

Session B6

METAL COMBUSTION FOR SUSTAINABLE ENERGY APPLICATION (TERRESTRIAN AND SPACE APPLICATIONS) II

Chair: H. Wang, Beijing University, Beijing, PRC

B24 GREEN IRON AND ALUMINUM AS RECYCLABLE ENERGY CARRIERS IN CIRCULAR ECONOMY

C. Hasse TU Darmstadt, D

B25 COMBUSTION OF METAL PARTICLES IN VARIOUS GASES – INVESTIGATION AND RECENT APPLICATION

V. Weiser

Fraunhofer ICT, Pfinztal, D

Bus transfer to hotels, Karlsruhe City and Main Station will be available (starting 19.00 h during the whole evening).

Friday, June 27

LECTURE ROOM A

Session A6

CHARACTERIZATION OF ENERGETIC MATERIALS USING AI/ML I

Chair: J. Pachman, University of Pardubice, CZ

09.00 A26 PREDICTING PROPELLANT HEAT FLOW CALORIMETRY TIMESERIES WITH MACHINE LEARNING

O. Schoenmakers, B. Mortier, W. Boon, S. de Koster TNO, NL

09.20 A27 MACHINE LEARNING METHODS FOR ANALYSING DAMAGE IN ENERGETICAL GRANULAR MATERIALS

C. Robin, F. Willot, P. Dokladal

Centre de Morphologie Mathematique, Mines Paris, F

S. Belon, E. Kaeshammer

CEA, Gramat, F

L. Borne, E. Fousson

ISL, Saint-Louis, F

09.40 A28 DEFECT CHARACTERISATION IN ICT SCANNED ENERGETIC MATERIALS USING MACHINE LEARNING

L. Green, R. Jones, A. Milroy QinetiQ, Farnborough, UK

10.00 A29 RESEARCH ON THE PREDICTION OF MECHANICAL PROPERTIES OF ENERGETIC MATERIALS USING MACHINE LEARNING TECHNIQUES

Wang Donglei, Yuan Hongwei, Liu Xuwang, Pang Haiyan

Institute of Chemical Materials CAEP, Sichuan, PRC

10.20 Coffee Break

Session B7

MUNITIONS IN THE SEA

Chair: A. Keßler, Fraunhofer ICT

B26 EUROPEAN RESEARCH AND INNOVATION ADDRESSING UNDERWATER MUNITION

T. Kiefer, J. Kandziora, P. Trautendorfer JPI Oceans, Brussels, B A. Keßler Fraunhofer ICT, Pfinztal, D

B27 AMMUNITION IN SWISS LAKES: HISTORY, INVESTIGATIONS AND CURRENT SITUATION

A.-L. Gassner, S. Pasche armasuisse, CH

B28 NATO STUDIES ON SEA-DUMPED MUNITIONS

A. S. Cumming University of Edinburgh, UK

B29 DEVELOPMENT AND CONSTRUCTION OF AN INDUSTRIAL PLANT FOR THE DISPOSAL OF MUNITIONS AT SEA

W. Sichermann Seascape GmbH, Hamburg, DE

Session A7

HIGH EXPLOSIVES

Chair: U. Schaller, Fraunhofer ICT

11.00 A30 EXPERIMENTAL DATA REQUIRED FOR
CALIBRATION OF REACTIVE BURN MODELS
IN PREDICTIVE EXPLOSIVE SIMULATIONS

J. D. Olles, A. F. Haslam, P. A. Fasano, C. D. Woodruff, R. T. Ichiyama, J. R. White

NSWC, Indian Head, USA

11.20 A31 SURVIVABILITY OF EXPLOSIVES WITH DYNAMICALLY COLLAPSING CAVITIES

J. Felts

NSWC, Indian Head, USA

H. Sandusky

Energetics Technology Center, Indian Head, USA

11.40 A32 tba

| 12.00 Awards and Closing Remarks | |
|----------------------------------|--|
| 12.20 Lunch | |
| 13.45 End of Conference | |

Session B8 PROPELLANTS

Chair: H. Östmark, FOI, SE

B30 NUMERICAL ANALYSIS OF MICROSCALE COMBUSTION PHENOMENA IN COMPOSITE SOLID ROCKET PROPELLANTS

P. Pietrek, M. Moroff Fraunhofer ICT, Pfinztal, D

B31 SAFETY AND PERFORMANCE EVALUATION OF A NEW HIGH-PERFORMANCE MONOPROPELLANT FORMED OF MICROENCAPSULATED FUELS IN COMBINATION WITH HYDROGEN PEROXIDE

R. Scholl, D. Freudenmann, S. Schlechtriem DLR. Hardthausen, D

B32 SYNTHESIS, CHARACERIZATION AND COMPARATIVE ANALYSIS OF THREE ENERGETIC PLASTICIZERS EXPLORING THE IMPACT OF DIVERSE FUNCTIONAL GROUPS ON PROPERTIES AND PERFORMANCE

J. T. Lechner, T. B. Keicher Fraunhofer ICT, Pfinztal, D

Poster Program

Posters will be presented during the whole Conference.

A special **Poster Session** will take place on **Thursday, June 26, 14.00 – 15.00 h**. During this time authors should be present for discussion at their posters in the foyer of the Conference Hall.

P1 PREDICTING THE THERMAL DEGRADATION OF ENERGETIC POLYMERS BY MEANS OF ARTIFICIAL NEURAL NETWORKS

M. Ticherfatine Ecole Nationale Superieure des Technologies Avancees, Algiers,

P2 EXPLORING THE IMPACT OF ENERGETIC POLYSACCHARIDE DOPANTS ON HTPB-PROPELLANTS PERFORMANCE USING NASA-CEA SIMULATION

M. Jouini, D. Trache, A. Abdelaziz, A.F. Tarchoun Ecole Militaire Polytechnique, Algiers, ALG

P3 PRINCIPAL COMPONENT ANALYSIS (PCA) OF DSC DATA: CRAFTING A UNIVERSAL PREDICTIVE MODEL FOR THE EQUIVALENT IN-SERVICE-TIME OF DOUBLE BASE ROCKET PROPELLANTS

- S. Chelouche, D. Trache, A.F. Tarchoun, A. Abdelaziz,
- S. Bekhouche

AIG

Ecole Militaire Polytechnique, Algiers, ALG

P4 ACCELERATING DISCOVERY OF FLUORINE-BASED ENERGETIC POLYMERS THROUGH MACHINE LEARNING AND DENSITY FUNCTIONAL THEORY

Siyan Deng, Serene Hay Yee Chan, Huey Hoon Hng Nanyang Technological University, Singapore, SGP

P5 EXPLORING THE EFFECTS OF NITROCELLULOSE-COATED NCUO ON THE THERMAL PROPERTIES AND KINETIC SIMULATION BEHAVIOR OF AMMONIUM NITRATE-BASED SOLID COMPOSITE PROPELLANTS WITH POLYURETHANE/ NITROCELLULOSE BLEND BINDERS

M. Nourine, M.K. Boulkadid, S. Touidjine, H. Akbi, S. Belkhiri Ecole Militaire Polytechnique, Algiers, ALG

P6 THE ROLE OF OXYGEN AND MOISTURE IN THE CHEMICAL COMPATIBILITY OF A NITRATE ESTER

E. Glascoe, C. Cockreham, J. Rosener, S. Hawks Lawrence Livermore National Laboratory, USA

P7 TOPOGRAPHIC INVESTIGATIONS OF VARIOUS HMX GRADES

M. Herrmann, H. Weyrauch Fraunhofer ICT, Pfinztal, D

P8 HIM_30: DESIGN AND EVALUATION OF A METAL-FREE HYPERGOLIC BIPROPELLANT BASED ON IONIC LIQUIDS AND HYDROGEN PEROXIDE

S.C. Stölzle, D. Freudenmann DLR, Hardthausen, D

P9 XPDFSUITE – A TOOL COLLECTION FOR THE PAIR DISTRIBUTION FUNCTION ANALYSIS (PDF)

P.B. Kempa, M. Herrmann Fraunhofer ICT, Pfinztal, D

P10 INVESTIGATION OF BU NENA IMPACT ON THE SENSITIVITY OF GUN PROPELLANTS

J. Ehrhardt, J. Glorian, B. Baschung ISL. Saint-Louis. F

P11 ASSESSMENT OF THE INTERACTION BETWEEN AMMONIUM DINITRAMIDE (ADN) AND A TRIAZINE BONDING AGENT FOR APPLICATION ON TECHNOLOGIES OF COMPOSITE SOLID PROPELLANTS

J.O. Silva, J.R.C. Silva, K.P. Cardoso, L.F.A. Ferrao Instituto Tecnologico de Aeronautica ITA, Sao Jose dos Campos, BR M.F. Diniz, M.Y. Nagamachi Instituto de Aeronautica e Espaco IAE, Sao Jose dos Campos, BR

P12 AI AND MACHINE LEARNING FOR PREDICTING QUANTUM TUNNELING EFFECTS IN ENERGETIC MATERIALS

Zihao Guo School of Chemical Engineering NJUST, Nanjing, PRC

P13 EXPLORING THE SOLVENT-BASED MANNICH REACTION FOR DESIGNING HIGH-PERFORMANCE BENZOXAZINE

S. Abdous, M. Derradji, K. Khiari, O. Mehelli, H. Abdelmalek Ecole Militaire Polytechnique, Algiers, ALG

P14 HIGH SPATIAL AND TEMPORAL RESOLUTION SENSORS BASED ON GAS IONIZATION: APPLICATION TO THE STUDY OF ENERGETIC BINDER

L. Jumpertz, L. Borne, F. Lutz, F. Schlesser, E. Fousson ISL, Saint Louis, F

P15 INVESTIGATING THE IMPACT OF GREEN NANO-METAL OXIDES (COPPER AND IRON) ON THE THERMAL DECOMPOSITION BEHAVIOR OF ADVANCED PROPELLANTS WITH NITROCELLULOSE/POLYURETHANE BINDERS

B. Rebiba, S. Touidjine Ecole Militaire Polytechnique, Algiers, ALG

P16 HOW CAN MOMENTUM TRANSFERS IN A BURNING MIXTURE OF AL/CUO PARTICLE POWDER BE MODELLED?

H. Magliano, D. Gauchard, A. Esteve, C. Rossi LAAS-CNRS University of Toulouse, F O. Simonin, P. Fede IMFT University of Toulouse, F

P17 VIBRATION-INDUCED DEGRADATION OF THE MECHANICAL PROPERTIES OF COMPOSITE ROCKET PROPELLANTS

M. Ferrapontoff Lemos, J.G. Passos Rodrigues, F. Santos da Luz Brazilian Navy Research Institute, Rio de Janeiro, BR M. Heil, M. Bohn Fraunhofer ICT, Pfinztal, D

P18 STUDY ON CATALYST-FREE CLICK REACTIVITY, IMPACT SENSITIVITY AND MIGRATION RESISTANCE OF GAP-BASED PU BINDERS WITH REACTIVE SPIRANE PLASTICIZERS

Mingyang Ma, Younghwan Kwon Daegu University, Gyeongsan, ROK

P19 EED IGNITION IN RELATION TO RADAR PEAK AND AVERAGE POWER

R.H.B. Bouma, A.P.M. Zwamborn, E.J. Kroon TNO, The Hague, NL

P20 SUBSCALE COMBUSTION TESTING AND MODELING OF ENCAPSULATED NITRATE ESTERS AS IGNITERS

D.T. Bird, C.A. Houthuysen
US Army DEVCOM, Picatinny Arsenal, USA

P21 CALCULATION OF LENNARD-JONES PARAMETERS BY DENSITY FUNCTIONAL THEORY CALCULATIONS

A. Omlor Fraunhofer ICT, Pfinztal, D

P22 MOLECULAR SIMULATION OF REACTION MECHANISMS AND TRANSITION STATES

A. Omlor, M. Bohn Fraunhofer ICT, Pfinztal, D

P23 CHEMICAL STABILITY OF THE CHNO-OXIDIZER TNEF

M.A. Bohn, J. Lechner, M. Heil Fraunhofer ICT, Pfinztal, D T.M. Klapötke Ludwig-Maximilian-University, München, D

P24 CAN MACHINE LEARNING HELP TO IMPROVE STABILITY OF ENERGETIC MATERIALS?

M. Heil, J. Langer, C. Fuchs, A. Kamienska-Duda, M. Szkudlarek Fraunhofer ICT. Pfinztal. D

P25 SOLUBILITY BEHAVIOR OF THE CL-20-MDNT COCRYSTAL SYSTEM AND IMPROVED SENSITIVITY THROUGH VACUUM EVAPORATIVE CRYSTALLIZATION

E. Wegert, P. Schultz Fraunhofer ICT, Pfinztal, D

P26 DEVELOPMENT AND VALIDATION OF A NUMERICAL MODEL FOR MULTI-MATERIAL SOLID ROCKET MOTORS

M. Moroff Fraunhofer ICT, Pfinztal, D

P27 MODELLING THE BURN RATE OF THERMITES WITH A DOE APPROACH

W. Becker, S. Knapp, D. Bieroth Fraunhofer ICT, Pfinztal, D

P28 COMBUSTION OF IRON PARTICLES IN OXYGEN AND AIR AS A REGENERATIVE ENERGY CARRIER ON EARTH AND THE MOON

V. Weiser, P. Pietrek, S. Knapp, S. Kelzenberg, M. del Mar Juez-Lorenzo, C. Seidel, D. Bieroth Fraunhofer ICT, Pfinztal, D

P29 NUMERICAL STUDY OF MULTI-MATERIAL SOLID ROCKET MOTORS FEATURING COMPLEX GRAIN STRUCTURES

M. Hausmann Fraunhofer ICT, Pfinztal, D

P30 OBSERVATION OF DECOMPOSITION OF AMMONIUM DINITRAMIDE BY MEANS OF X-RAY DIFFRACTION

C. Seidel, M. Herrmann Fraunhofer ICT, Pfinztal, D

P31 FIRST SYNTHESIS OF AN ENERGETIC DIACRYLATE FOR ADVANCED 3D PRINTING OF ENERGETIC MATERIALS

H. Wegner, A. Mendl, D. Boskovic, U. Schaller Fraunhofer ICT, Pfinztal, D

P32 IMPROVING THE MECHANICAL PROPERTIES OF 3D PRINTED GUN PROPELLANTS

D. Mitro, A. Dresel Fraunhofer ICT, Pfinztal, D

P33 EXPERIMENTAL AND NUMERICAL INVESTIGATION OF DIFFERENT DETONATORS IN TERMS OF THE INITIATION STIMULUS

T. Heidebrecht, C. Zimmermann Fraunhofer ICT, Pfinztal, D

P34 BLAST SIMULATION: THERMAL AND MATERIAL ANALYSIS

M. Lasota, T. Heidebrecht, C. Zimmermann, S. Wurster Fraunhofer ICT, Pfinztal, D

P35 INVESTIGATION ON PHYSICS AWARE NEURAL NETWORKS FOR THE DETERMINATION OF DETONATION PARAMETERS OF NON-IDEAL EXPLOSIVES

D. Tomaschewski, F. Steinhauser Fraunhofer ICT, Pfinztal, D

P36 HITDOC – THE FIRST EDF TECHNOLOGICAL CHALLENGE, ADDRESSING TECHNOLOGIES FOR THE DETECTION OF LANDMINES AND IMPROVISED EXPLOSIVE DEVICES (IEDS)

I. Wilhelm, F. Schnürer Fraunhofer ICT, Pfinztal, D H. Önnerud, D. Letalick FOI, SE D. Deiana, M. Koolloos TNO, NL

J.J. Navlet Salvatierra, J.M. Gomez Sanz INTA, ES

P37 SEMI-AUTOMATED SPECTRAL QUANTIFICATION OF THE CONCENTRATION OF INGREDIENTS IN GUN PROPELLANTS

J. Langer, M. Heil, C. Fuchs Fraunhofer ICT, Pfinztal, D

P38 DUMPED AMMUNITION – A CHALLENGE FOR ARTIFICIAL INTELLIGENCE FOR THE 21st CENTURY

T. Salacinski, M. Szala, B. Wiaderek, K. Rzadkowska Military University of Technology, Warsaw, PL

P39 HIGH-ENERGY BALL MILLING: AN ALTERNATIVE TECHNIQUE FOR PREPARING REACTIVE NANOPOWDERS

P.-H. Esposito, R. Denoyel, M.-V. Coulet Aix-Marseille University CNRS, Marseille, F

P40 PARAMETRIC MODELLING OF COMPLEX AGEING BEHAVIOR OF TENSILE MODULUS IN CTPB-BONDED PROPELLANT

M.A. Bohn Fraunhofer ICT, Pfinztal, D G.S. Tussiwand HAPTICA s.r.l., Busto Arsizio, IT

P41 FLASHPOINT PREDICTION

T. Wombacher, K. Lehmann Merck Life Science, Darmstadt, D

P42 EFFECT OF CARBON NANOTUBES ON THERMAL DECOMPOSITION OF CL-20 EXPLOSIVE: A MOLECULAR DYNAMICS SIMULATION STUDY

Shupei Zhang, Danyang Liu, Kun Yang, Jianying Lu, Lixiang Zhong, Junying Wu, Lang Chen Beijing Institute of Technology, Beijing, PRC

P43 SYNTHESIS AND APPLICATION OF HIGH IRON CONTENT FERROCENE DERIVATIVE POLYMER AS COMBUSTION CATALYST

Mushuang Qian, Xiaoqiang Li, Jiaxin Liu, Jun Yang Shanghai Institute of Organic Chemistry (CAS), Shanghai, PRC

P44 ENERGETIC MATERIALS BASED ON PARAFFIN USED IN A SPACE INDUSTRY AS FUELS FOR HYBRID ROCKET ENGINES

B. Smetana, M. Kawulokova, S. Zla, P. Dostal, H. Matuskova, J. Dobrovska

Technical University of Ostrava, Ostrava-Poruba, CZ C. Boros

Borospace s.r.o., Bratislava, SK

P45 THE STUDY ON THE STABILITY OF HAN BASED GEL PROPELLANT

Jun Yang, Hui Li Shanghai Institute of Organic Chemistry (CAS), Shanghai, PRC

P46 A COMPREHENSIVE INVESTIGATION INTO SAFETY AND YIELD FOR SYNTHESIS OF LOW-SENSITIVITY HIGH EXPLOSIVE 3-NITRO-1,2,4-TRIAZOL-5-ONE

M. Elnegoumy, C. Dubois, E. Comtois Ecole Polytechnique de Montreal, CAN A. Elbeih Military Technical College, Cairo, ET

P47 THERMODYNAMIC CRITERIUM FOR EXPLOSIVE MATERIALS AND DETONATIVE REACTIONS

E.-C. Koch

Lutradyn Energetic Materials, Kaiserslautern, D

P48 TERNARY THERMITES: INFLUENCE OF MIXING RATIO ON THERMITE REACTIONS

E. Roth, S. Knapp, A. Raab Fraunhofer ICT, Pfinztal, D

Notes

Notes

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55th International Annual Conference of the Fraunhofer ICT

June 23-26, 2026 Convention Center Karlsruhe, Germany

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Conference Management

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