The Reductionism/Holism Conundrum

Indaba 10

11 – 16 October 2026

Skukuza, Kruger National Park, South Africa

PROGRAM

Sunday 11 October 2026

14:00 – 18:00	**Registration**	*Nombolo Mdhluli Conference Centre*
18:30	**Welcoming function**	*Boma*

Monday 12 October 2026

05:30	**Game viewing** Delegates using conference transport will leave from the conference centre; delegates with their own transport make their own arrangements.
From 07:00	Breakfast — *Cattle Baron Restaurant*
08:30 – 08:45	**Welcoming** Andreas Roodt *Chair of the INDABA 10 Organising Committee*
	Session 1 **Chair: Alessia Bacchi**
08:45 – 09:15	**Materials for Sustainability: Photo(electro)catalysis and Adsorption** Santiago Garcia-Granda *University Oviedo, Spain*
09:15 – 09:45	**Mixed ligand Cu(II) coordination polymers: architecture–stability relationships from crystallography, VT PXRD and desolvation kinetics** Susan Bourne *University of Cape Town, South Africa*
09:45 – 10:15	**Dynamic Processes in Crystalline Coordination Polymers** Marijana Đaković *University of Zagreb, Croatia*
10:15 – 11:00	**Refreshments** All posters to be mounted
	Session 2 **Chair: Roger Alberto**
11.00 – 11:20	**From Poultry to Pillows: Navigating Structural Control and Scale-Up Hurdles of Small Molecules for Global Nutrition and Health** Marietjie Schutte-Smith *University of the Free State, South Africa*
11.20 – 11:40	**Bragg versus Total Scattering: A Variable Temperature Bi_2O_3-based Case Study** Caren Billing *University of the Witwatersrand, South Africa*
11.40 – 12:00	**Catalysis-like Protein Transfer Enables Stable Histidine-Tag Immobilization on Liposomal Membranes** Leon Hermann *Max Planck Institute for Medical Research, Germany*



12.00 – 12:30	**Adventures in the Vast Transition Metal Chemical Space** Angelo Frei *University of York, United Kingdom*
12.30 – 12:50	**Predictability and Emergence in Organic Solid-State Reactions: From Schmidt's Criterion to Cooperative Transition States** Manuel Fernandes *University of the Witwatersrand, South Africa*
13:00 – 14:00	**Lunch** *Amukelekani Restaurant*
	Session 3 **Chair: Susan Bourne**
14.00 – 15:00	**Poster flash presentations** (2 minutes each)
15.00 – 16:00	**Poster Session**
16.00 – 17:45	**Game viewing**
17:45	**Cocktail function at Skukuza Golf Club** All delegates to convene in front of conference centre for transport to the Skukuza Golf Club. NO private cars allowed

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05:30	**Game viewing**
From 07:00	**Breakfast** *Cattle Baron Restaurant*
	Session 4 **Chair: Catharine Esterhuysen**
08.15 – 08:45	**From Liquid Ingredients to Crystalline Smart Materials** Alessia Bacchi *University of Parma, Italy*
08.45 – 09:15	**Dynamic Behaviour in Porous Crystalline Materials** Lee Brammer *University of Sheffield, United Kingdom*
09.15 – 09:45	**Multicomponent Crystals from the Gas Phase** Delia Haynes *Stellenbosch University, South Africa*
09.45 – 10:15	**The Menstrual Safety Conundrum: Navigating Vaginal Permeability, Environmental Persistence and Period Poverty in Search for "Sufficient" Science** Deon Visser *University of the Free State, South Africa*
10:15 – 10:45	**Refreshments**
	Session 5 **Chair: Radosław Kamiński**
10.45 – 11:15	**You are the Chemist. Validate our Process.** Johannes Van Tonder PET Labs Pharmaceuticals
11.15 – 11:45	**Decoding 'Unnatural' Metal-Protein Coordination – is Best Data, Good Enough for Life?** Alice Brink *University of the Free State, South Africa*
11.45 – 12:15	**Rational Design of Rhenium(I) Metallotherapeutics from Molecular Precision to Targeted Theragnostics** Orbett Alexander *University of the Western Cape, South Africa*
12.15 – 12:45	**Investigating Mechanisms of Iridium Hydrides in Dehydrogenation and Carbon Dioxide Activation. Chemistry for Sustainability or Rather Only Curiosity Driven Research?** Ola Wendt *Lund University, Sweden*
12:45	**Group picture**
13:00	**Lunch** *Amukelekani Restaurant*
14:00	**Game viewing**



From 18:30	**Dinner** – own arrangements
	Session 6 **Jan Boeyens Session** **Chair: Peter Comba**
19:30 – 20:00	**Numbers in Crystals and Matter. *The Holistic Science of Jan C.A. Boeyens*** Demi Levendis *University of the Witwatersrand, South Africa*
20:00 – 20:30	**Carbofuran Crystal Polymorphic Form for Efficient Malaria Vector Control** Andreas Lemmerer *University of the Witwatersrand, South Africa*
20:30 – 21:00	***Jan Boeyens Award Lecture*** **The Reductionism–Holism Conundrum in Medicinal Organometallic Chemistry: From Structure and Speciation to Biological Function** Andrew Swarts *University of the Witwatersrand, South Africa*

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Wednesday 14 October 2026

05:30	**Game viewing**
From 07:00	**Breakfast** *Cattle Baron Restaurant*
	Session 7 **Chair: Delia Haynes**
08.15 – 08:45	**Oxidation State Changes in Reactions of Molecular Gold Complexes: From Formal to Physical Principles** Johannes Klein *University of Groningen, The Netherlands*
08.45 – 09:15	**"Everything Should be Made as Simple as Possible, but Not Simpler": Balancing Reductionism and Realism in Density Functional Theory Models** Jeanet Conradie *University of the Free State, South Africa*
09.15 – 09:45	**Protein Crystallography in the Age of AlphaFold2: When Enough is not Enough** Elspeth Garman *University of Oxford, United Kingdom*
09.45 – 10:15	**Photo- and High-Pressure Crystallography of D^8/D^{10} Transition-Metal Complexes - In Search of Structure-Property Relationships** Katarzyna Jarzembska *University of Warsaw, Poland*
10:15 – 10:45	**Refreshments**
	Session 8 **Chair: Orbett Alexander**
10.45 – 11:15	**Activation of Small Molecules: Can Boron act as a Transition Metal?** Holger Braunschweig *Julius-Maximilians-University of Würzburg, Germany*
11.15 – 11:45	**Activation of Small Molecules: Can Transition Metal Compounds act as a Main Group Species?** Sven Schneider *University of Göttingen, Germany*
11.45 – 12:15	**Activation of Small Molecules: Theoretical (Ad)Ventures and Frontiers** Max Holthausen *Goethe University, Germany*
12.15 – 12:45	**Lanthanide-Dependent Metalloproteins and Biomimetics: What We can Learn from Models about the Bioinorganic Chemistry of Lanthanides** Lena Daumann *Heinrich-Heine Universität Düsseldorf, Germany*
13:00	**Lunch** *Amukelekani Restaurant*
14:00	**Game viewing**
Evening	**Dinner** – own arrangements

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Thursday 15 October 2026

06:00	**Game viewing**
From 07:00	**Breakfast** *Cattle Baron Restaurant*
	Session 9 **Chair: Elspeth Garman**
08.15 – 08:45	**Unravelling the Real Structure of Solid Oxide Electrolytes** Dave Billing *University of the Witwatersrand, South Africa*
08.45 – 09:15	**The Continuum of Covalent Contributions to Noncovalent Interactions** Catharine Esterhuysen *Stellenbosch University, South Africa*
09.15 – 09:45	**Topochemistry for Solving Challenges in Polymer Synthesis** Kana Sureshan *IISER Thiruvananthapuram*
09.45 – 10:15	**Into the Crystal Wild: When and Why Solvates Form** Aurora Cruz-Cabeza *Durham University, United Kingdom*
10:15 – 11:00	**Refreshments** Posters to be removed
	Session 10 **Chair: Marijana Đaković**
11:00 – 11:20	**Redefining Laboratory Crystallography: High-Intensity Silver Radiation and Advanced Detection for Precision Structural Analysis** Pratha Jagannatha *Bruker India Scientific Pvt. Ltd, India*
11.20 – 11:50	**Functional Molecular Vessels** Partha Mukherjee *Indian Institute of Science*
11.50 – 12:20	**Combining Quantum Chemistry and Machine Learning for Catalyst Design in Small-Molecule Activation** Gopalan Rajaraman *Indian Institute of Technology Bombay, India*
12.20 – 12:50	**Small Molecule Activation at Transition Metal Centers: Structure-Function Correlations** Kallol Ray *Humboldt-Universität zu Berlin, Germany*
13:00 – 14:00	**Lunch** *Amukelekani Restaurant*
	Session 11 **Chair: Andreas Roodt**
14:30 – 15:00	***De Novo* Designed Miniproteins** Franziska Thomas *Heidelberg University, Germany*

15.00 – 15:30	**Modeling spin for applications of metal complexes** Peter Comba *Heidelberg University, Germany*
15:30 – 16:00	**Closing**
17:00	**Conference dinner** Game drive & bush braai All delegates to convene at parking area in front of conference centre

Friday 16 October 2026

From 07:00	**Breakfast** *Cattle Baron Restaurant*
09:00	**Departure**

POSTERS

1 **Spectroscopic Studies on the Coordination Behavior of Functionalized Phenanthroline Ligands**
Dolapo Ashiru
University of South Africa, South Africa

2 **Investigating The Cytotoxic and Apoptotic Effects of Rotenone in Triple-Negative Breast Cancer Cells**
Pearl Doe-Thompson
University of Ghana, Ghana

3 **Two Tales from One Bacterium: Carotenoid Biosynthesis and Lanthanide and Iron Metabolism in *Methylobacterium extorquens* PA1**
Pia Heinrichs
Heinrich Heine University, Germany

4 **Exploration of Physical, Chemical and Biological Properties of Group 6 and 7 Tricarbonyl Complexes with Tridentate Bis-Quinoline Ligands**
David Husbands
York University, United Kingdom

5 **Crystallography and cell testing - integrating interdisciplinary strengths to evaluate structure-activity relationships for radiopharmaceutical development**
Francois Jacobs
University of the Free State, South Africa

6 **pH-Controlled Iron(III) Hydroxide Incorporation into *Acacia mearnsii* Carbon Composites for Tetracycline Remediation**
Elham Jalali
University of the Free State, South Africa

7 **Understanding Molecular Structures in Chemical Engineering and Medicinal Applications Through SC-XRD**
Dumisani Kama
University of the Free State, South Africa

8 **Synergistic Evaluation of Sulfonamide Ligands using the "2 + 1" Coordination Approach of Re^{I}-Tricarbonyl Complexes with Effective Monodentate Ligands**
Mmabatho Ledibane
University of the Western Cape, South Africa

9 **Cannabis Sativa Active Compounds: Isolation, Characterisation and Study of their Entourage Effect on HIV, Anticancer and Antioxidant**
Sachedi Machedi
Vaal University of Technology, South Africa

10 **Mixed-Ligand Complexes of Lanthanides Derived from an A-Hydroxycarboxylic Acid (Benzilic Acid) and 1,10-Phenanthroline: Physicochemical Properties and Anticancer Activity**
Tatenda Madanhire
University of South Africa, South Africa

11 **Structural, DFT, Molecular Docking and Cytotoxicity Studies of the Dibromido (H^{6}-*P*-Cymene) (Triphenylphosphine) Ruthenium(II) Complex**
Ferdinand Misakabu
University of South Africa, South Africa

12 **Investigating Structure-Activity Relationships in Rhenium(I) Phosphine Complexes with Anticancer Activity**
Lehlohonolo Motsieloa
University of the Western Cape, South Africa

13 **Synergistic Immunity: Unraveling NK and γδ T Cell Collaboration in Cancer**
Deus Mwesigwa
Max Planck Institute for Medical Research, Germany **Pine Biochar for Efficient Atrazine**

14 **Removal from Contaminated Water**
Matin Naghizadeh
University of the Free State, South Africa

15 **Structural Modification of Isoniazid via Schiff Base Formation and Rhenium(I) Coordination for Enhanced Antitubercular Activity**
Jordan Ncube
University of the Western Cape, South Africa

16 **Re(I)-Tricarbonyl Complexes with Pyrazolyl-Based Ligands as Potential Antibiotic Metallo-Drugs**
Boitumelo Nthapo
University of the Western Cape, South Africa

17 **Molecular Design and Biological Activity of Re(I) Tricarbonyl Complexes**
Lesetja Ramoba
Tshwane University of Technology, South Africa

18 **Crystal structure analysis of dichlorido(η^6-*p*-cymene)(triphenylstibine) ruthenium(II)**
Rufaro Razuwika
University of South Africa, South Africa

19 **Valorization of Agricultural Waste: Spent Black Wattle Bark to Superabsorbent Polymers**
Christine Rossouw
University of the Free State, South Africa

20 **Design and Development of Rhenium(I) Tricarbonyl Polypyridyl Complexes for Biological Applications**
Brithney Snyman
University of the Western Cape, South Africa

21 **Half-Sandwich Metallacycles of Ru(II) and Os(II) with Asymmetric Diphosphine Selenide Ligand: Experimental and Theoretical Studies**
Kgaugelo Tapala
University of South Africa, South Africa

22 **Insights into the Structural Analysis of Caffeine–Oxalic Acid Co-crystals Using High-Resolution PXRD and Computational Refinement**
Sihle Thabethe
University of Cape Town, Suth Africa

23 **From Metal Complexes to Wildlife Mysteries: A Journey of a Lost Crystallographer**
Christo van Staden
University of the Free State, South Africa

24 **Structural Dynamics of Simple Organic and Soft Porous Crystals**
Banele Vatsha
University of Johannesburg, South Africa

25 **Rational Design and Synthesis of Eco-Responsive Schiff Base Ligands for Selective Chelation and Recovery of Heavy Metal Ions**
Nondumiso Zwane
Department of Chemistry, South Africa