

Session Program

1-3 Dec 2026



International Meeting on

Theoretical and Experimental Chemistry:

How to Design and Study
New Compounds with
Potential Application

International Meeting on Theoretical and Experimental Chemistry: How to Design and Study New Compounds with Potential Application

Session 3. Chair: Aneta Jezierska

Wrocław, Poland, WEBINAR (ONLINE CONFERENCE, FREE OF CHARGE, time zone: CET, UTC+1)
ul. F. Joliot-Curie 14 50-383 Wrocław, Poland

Wednesday 2 December

11:00

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Session |**Location:** Wrocław, Poland, WEBINAR (ONLINE CONFERENCE, FREE OF CHARGE, time zone: CET, UTC+1), ul. F. Joliot-Curie 14 50-383 Wrocław, Poland

11:00–11:30

Reactivity Indices from Conceptual Density Functional Theory: Analytical and Data-Based Evaluation and Extension to Excited States

Speaker

Prof. Frank De Proft

11:30–12:00

Scientific Research in the Digital Era - Quo Vadis?

Speaker

Mrs Agnieszka Szymańska-Kwiecień

12:00–12:30

Building the QUEST database: the computational and chemical challenges of obtaining reference excited-state data

Speaker

Prof. Denis Jacquemin

12:30–13:00

Modelling the Lowest Triplet States of Cu(I) Photosensitizers

Speaker

Prof. Marcin Andrzejak

13:00