



Wrocław  
University  
of Science  
and Technology

# Modeling and Design of Molecular Materials 2025

Wrocław, Poland, September 7–11, 2025

## 10-th MDMM conference organized

by Wrocław University of Science and Technology

### Conference topics

This interdisciplinary meeting will be devoted to presenting contemporary computational methods along with their applications in molecular modeling, molecular material design, bioinformatics and related fields. Participation of experimentalists interested in application of molecular modeling techniques is encouraged. The following topics will be covered:

- applications of machine learning
- advances in computational methods
- modeling chemical reactions and catalysts
- modeling biomolecules
- modeling electronic structure
- modeling molecular materials

### Proceedings

Refereed conference contributions will be published in Journal of Molecular Modeling (Springer Nature).

<https://link.springer.com/journal/894/updates/27727658>

Springer Nature will also sponsor prizes in the best student poster contest.

### Honorary Scientific Committee

- T. Andruniow (CHAIR) — Wrocław Tech, Poland
- J. Burda — Charles University, Prague, Czech Republic
- T. Clark — Erlangen-Nurnberg University, Germany
- A. Eilmes — Jagiellonian University, Poland
- J. Korchowiec — Jagiellonian University, Poland
- J. Rak — Gdańsk University, Poland
- P. Rutkowski — Dean of the Faculty of Chemistry, Wrocław Tech, Poland
- W. A. Sokalski — Wrocław Tech, Poland
- R. Wieczorek — University of Wrocław, Poland

### Sponsors

- Faculty of Chemistry, Wrocław University of Science and Technology
- Springer Nature

### Confirmed invited speakers

- H. Agren — Wrocław Tech, Poland
- J. Burda — Charles Univ, Czech Republic
- T. Cierpicki — Univ Michigan, USA
- P.O. Dral — Xiamen Univ, China
- A. Eilmes — Jagiellonian Univ, Poland
- J. Grembecka — Univ Michigan, USA
- B. Grzybowski — UNIST, South Korea
- J. Harvey — KU Leuven, Belgium
- P. Imhof — Univ Erlangen, Germany
- O. Isayev — Carnegie Mellon Univ, USA
- J. Korchowiec — Jagiellonian Univ, Poland
- Z. Lan — South China Normal Univ, China
- K. M. Langner — Google Deep Mind, USA
- A. Michalak — Jagiellonian Univ, Poland
- T. Martinez — Stanford Univ, USA
- V. Moliner — Castellon, Spain
- P. Piecuch — Michigan State Univ, USA
- J. Rak — Gdańsk Univ, Poland
- U. Ryde — Lund Univ, Sweden
- K. Szalewicz — Univ of Delaware, USA
- M. E Tuckerman — New York Univ, USA
- T. Wesolowski — Univ Geneva, Switzerland

### Contact details

Correspondence should be sent to:

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Detailed information, program and registration form will be available on the web page:

<https://mdmm.pwr.edu.pl>

### Important dates

- April 30, 2025 — Registration and early fee payment
- June 15, 2025 — Abstracts and late fee payment
- September 7–11, 2025 — Meeting



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<https://mdmm.pwr.edu.pl>