Modeling & Design of Molecular Materials 2025

Wrocław, September 7-11, 2025

Practical Guide & Information

Conference website: https://mdmm.pwr.edu.pl/

Wrocław University of Science and Technology
Rector's Honorary Patronage

Faculty of Chemistry

SPRINGER NATURE

Wrocław University of Science & Technology

REACHING THE CONFERENCE VENUE

The conference is being held at the **Wrocław University of Science and Technology (Wrocław Tech)** (`www.pwr.edu.pl`) in Lower Silesia, Poland. The conference venue is situated on the first floor of H-14 conference building (Wybrzeże Wyspiańskiego 40) opposite to the Main A-1 building in the middle of the university campus, close to the Grunwaldzki Square, (*Plac Grunwaldzki – Rondo Reagana* tram & bus stop).

Wrocław Copernicus Airport (WRO)

Services regular flights from Warsaw, Barcelona, Bologna, Frankfurt, Milan, Munich, etc. (see flight timetable: `http://www.airport.wroclaw.pl/en/`). Warsaw, Munich, or Frankfurt are usually the best choices for connecting flights. Bus number 106 (single ticket costs 4.60 zł) connects the airport with main railway station and departs every 15-20 minutes (the first departure on Sat/Sun: 5:21, the last one: 23:43). Taxi fare from airport to hotels is approximately 75-85 zł (15 to 20 EUR), and increases at night by ∼25%. Ask for an invoice to avoid fraud. Connections from Main Railway Station to conference venue are described below.

Railway and bus connections

Polish Railways (PKP) offer regular train connections to many major European cities as well as direct trains to the majority of big Polish cities. Refer to online timetables (`https://rozklad-pkp.pl/en`). **Wrocław Bus Station** can be found under the Wroclavia shopping center in the vicinity of the main railway station. To reach the city centre or Wrocław Tech, walk through the tunnel next to the railway station and use tram/bus connections.

Public transportation within Wrocław

Wrocław has a rich network of bus and tram connections. The following trams and busses can take you from the main railway station to the Grunwaldzki Square and WUST:

- Tram No. 4 (direction *Biskupin*, 6-7 stops to the Grunwaldzki Square).
- Tram No. 2 (direction *Biskupin*, 6 stops to the Grunwaldzki Square).
- Buses No. 145 (*direction Sepolno*) and 146 (*direction Bartoszowice*, 5-6 stops to Grunwaldzki Square)

Tickets: Single ride: 4.60 zł. Other options include a daily ticket, which costs 15.00 zł.[1,2] **Purchase:** You can select and buy a ticket on a terminal inside any bus or tram, and pay with your bank card. You *will not* get a ticket or receipt in such a case and the ticket inspector can check the validity by scanning your card, if you happen to come across one. If you buy a ticket in one of the ticket machines at a bus/tram stop, make sure to collect the paper ticket and validate it inside the bus or tram. Alternatively, you can buy a ticket via the SkyCash app, providing the 4-digit identification number of your vehicle, which can be found inside the vehicle (e.g. on the front or back wall).

[1] Polish and foreign students with proper ID (e.g. Polish Student ID or ISIC) can buy half-price tickets (2.30 zł)

[2] Other time-based tickets are also available (15 min: 3.20, 30 min: 4.00 zł, 60 min: 5.20 zł, 90 min: 7.00 zł, etc.). Remember to validate your ticket in case you buy the paper version from the machine.

ARRIVAL AND ON-SITE REGISTRATION

Upone arrival, participants should check-in at the registration desk **in the lobby of the H-14 building**, sign the attendance list, and collect their badges and conference materials including printed copy of this mini-guide containing detailed conference schedule, list of posters and a flash drive with the complete book of abstracts. Flash drives are equipped with USB-C connectors to enable viewing the contents using your smartphone. On Sunday, 7^{th} of September, you may also bring your poster to attach it to the boards and stands in the H-14 building. The registration desk will be open on Sunday, 7^{th} of September, from 14:00 to 18:00. Starting from Monday, 8^{th} of September, the registration desk will be opened 30 minutes before the first morning session and during coffee breaks near the entrance to the lecture hall in the H-14 building.

INTERNET ACCESS

On the Wrocław University of Science and Technology campus, participants will be able to access Wi-Fi networks through both **Eduroam** and **PWrGuest**. The QR code on the right can be used to connect with the PWrGuest Wi-Fi Network.
Detailed instructions for logging in and using these networks are available under the following links:
Eduroam: `https://di.pwr.edu.pl/uslugi/siec/eduroam`
PWrGuest: `https://di.pwr.edu.pl/uslugi/siec/pwrguest`

In the H-14 building, Internet access will also be possible via the H14Goscie Wi-Fi network, the password for which is: GosciePWR.

CONTRIBUTIONS AND CONFERENCE PROGRAM

Lectures

The conference program can be found in conference website and in the book of abstracts. Lecturers, please transfer your presentation to our technical personnel headed by dr Paweł Kędzierski via flash drive or email at the latest during the coffee break preceding the session in which your presentation is to be delivered. The presentations can only be saved as PPT, PPTX or PDF files. The supported format for video attachments is MP4 and for audio attachments is MP3 or WAV. Presentations should be prepared in 16:9 aspect ratio with full HD (1920x1080 px) resolution. Due to technical issues related to the digital screen operating system, sharing the presentation from your own laptop will only be possible via an HDMI connection and only if there are problems with exporting the presentation via a flash drive or email.

Posters

The posters should be prepared in A0 format and oriented vertically. The posters cannot be prepared in landscape orientation, as they will not fit in the stands. Poster boards will be available in the H-14 building from Sunday afternoon, 7^{th} of September. Poster presenters are asked to hang their posters on the stands no later than 16:00 on Monday, 8^{th} of September. The poster session is scheduled for 16:15 that day, and poster presenters are asked to remain at their posters during the session. A contest for the best posters presented by undergraduate and graduate students is planned. The posters must remain on their stands until Tuesday, 9^{th} of September, at 9:00 at the latest, so we kindly ask that you remove them yourself by then. They will then be removed by the organizing committee.

Conference proceedings

Refereed conference contributions will be published in Journal of Molecular Modeling (Springer Nature), IF = 2.5 (2024): https://link.springer.com/journal/894/updates/27727658.
The deadline to submit manuscripts for review will be around December 15, 2025. Proceedings from previous conferences can be found in the same journal.

LEISURE & ATTRACTIONS

- **Group photo** will be taken on the terrace of the H-14 building at 17:40 on Tuesday (9^{th} September), immediately after the coffee break following Session VII.
- **Wrocław sightseeing cruise** is planned for Wednesday (10^{th} September), 15:00–18:00. The cruise ship will depart from the marina near the H-14 building and will have two possible final stops: (1) the marina near the Wrocław ZOO, or (2) the marina in the City Centre. Participants may choose at which stop to disembark. This event is free of charge, but participants are kindly asked to sign up at the registration desk.
- **Conference banquet** will take place after the cruise (10^{th} September, 19:00–21:00) at the *La Maddalena* restaurant (1 Pomorska Street). Entry upon presentation of an individual invitation, which will be given to participants during check-in.

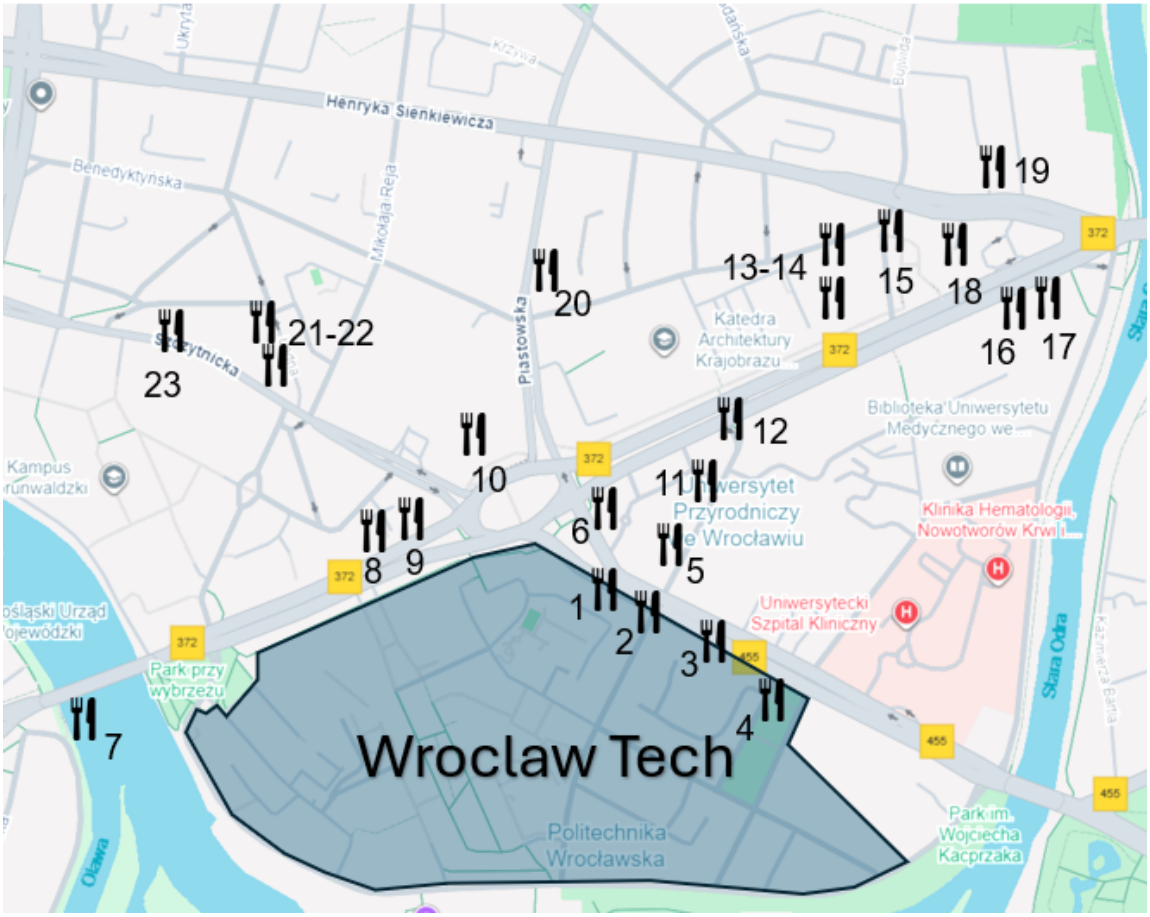
Other Attractions in Wrocław

- **Panorama of the Battle of Racławice** (11 J. E. Purkyniego Street) Open daily from 8:30 to 19:00. https://mnwr.pl/category/oddzialy/panorama-raclawicka/
- **National Museum** (5 Plac Powstańców Warszawy) Open Tuesday–Friday 10:00–17:00, Saturday–Sunday 10:30–18:00. https://mnwr.pl/category/oddzialy/muzeum-narodowe/
- **Four Domes Pavilion** (1 Wystawowa Street) Open Tuesday–Friday 10:00–17:00, weekends 10:00–18:00. https://mnwr.pl/category/oddzialy/pawilon-czterech-kopul/
- **Japanese Garden** (1 Adama Mickiewicza Street) Open daily from 9:00 to 19:00.
- **Wrocław Dwarfs** — an interesting way to discover the city is by searching for its small bronze inhabitants. You can find an interactive map in the mobile app: https://wroclaw.citygame.com.pl/
- **Kolejkowo - Wonderful world in miniature** (95 Powstańców Śląskich Street, I floor) Open daily from 10:00 to 18:00. https://kolejkowo.pl/wroclaw
- **Hydropolis - Centre of knowledge about water** (17 Na Grobli Street) Open Monday–Friday 10:00–18:00, Saturday–Sunday 10:00–20:00. https://hydropolis.pl/

RESTAURANTS NEAR CONFERENCE VENUE

1. **Greco Studio** (Greek) — Curie-Skłodowskiej 33. Mon–Sun 12:00–23:00. Vegan: Limited. Spacious venue. ∼5 min walk.
2. **El Gordito Grunwald** (Mexican/Tex–Mex) — Curie-Skłodowskiej 39/U1A. Mon–Sun 12:00–21:00. Vegan: Likely. Small venue. ∼5 min walk.
3. **Przegryź na Skłodowskiej** (Polish home–style) — Curie-Skłodowskiej 55/61. Mon–Fri 08:00–17:00. Vegan: Limited. Small venue. ∼5 min walk.
4. **Solleim** (Korean) — Łukasiewicza 18. Mon–Sun 11:00–22:00. Vegan: Yes. Small-sized venue. ∼5 min walk.
5. **Panda Ramen** (Japanese ramen/sushi) — Norwida 32. Mon–Sun 11:00–22:00. Vegan: Yes. Small/medium venue. ∼5 min walk.
6. **Starbucks** (Coffeehouse) — Plac Grunwaldzki 23. Mon–Sun 07:00–21:00. Vegan: Yes. Spacious café. ∼5 min walk.
7. **Odra Centrum** (Café/European) — Wybrzeże Juliusza Słowackiego 5B. Mon–Thu 10:00–21:00; Fri-Sun 10:00–01:00. Vegan: Yes. Medium café. ∼5 min walk.
8. **Bravo** (Italian pizzeria) — Plac Grunwaldzki 18/20. Mon–Sun 11:00–23:00. Vegan: Limited. Medium venue. ∼5 min walk.
9. **THALI** (Indian) — Plac Grunwaldzki 18/20. Mon–Sun 12:00–22:00. Vegan: Yes. Medium-sized venue. ∼5 min walk.
10. **Pasaż (McDonald's, KFC, Salad Story, etc.)** (Mixed fast food) — Within Pl. Grunwaldzki passage. Mon–Sun ∼10:00–22:00. Vegan: Limited. Large food court. ∼5 min walk.
11. **Cynamon Bar** (Mixed buffet) — Plac Grunwaldzki 23. Mon–Fri 08:00–17:00. Vegan: Limited. Medium canteen-style venue. ∼5 min walk.
12. **Domino's Pizza** (Pizza/fast food) — Plac Grunwaldzki 23/27. Mon–Sun 11:00–23:00. Vegan: Limited. Medium-sized venue, mostly takeaway. ∼5 min walk.
13. **WOO THAI** (Thai) — ul. Grunwaldzka 67. Mon–Sun 12:00–21:00. Vegan: Yes. Medium-sized venue. ∼10 min walk.
14. **Papi Chulo Cantina** (Mexican) — Grunwaldzka 67, Pasaż Niepolda. Mon–Thu 13:00–21:30; Fri 13:00–22:30, Sun 13:00–20:00. Vegan: Limited. Medium-sized venue. ∼10 min walk.
15. **Chingu** (Korean street food) — Bujwida 25. Mon–Sun 11:00–21:00. Vegan: Yes. Small venue. ∼10 min walk.
16. **Bella Storia** (Italian) — Pl. Grunwaldzki 53. Mon–Sun 10:00–24:00. Vegan: Limited. Medium-sized venue. ∼10 min walk.
17. **U Gruzina** (Georgian) — Pl. Grunwaldzki 59. Mon–Fri 12:00–00:00, Sat-Sun 10:00-20:00. Vegan: Limited. Medium size venue. ∼10 min walk.
18. **McDonald's** (Fast food) — Pl. Grunwaldzki 34. Mon–Sun 07:00–00:00. Vegan: Limited. Large venue. ∼10 min walk.
19. **Przyjaciele i Znajomi** (Polish gourmet) — Grunwaldzka 98. Mon–Sun 12:00–21:00. Vegan: Yes. Large restaurant. ∼10 min walk.
20. **Restauracja Asia** (Asian) — Piastowska 19. Mon–Sun 11:00–21:00. Vegan: Likely. Small venue. ∼15 min walk.
21. **Pho Viet** (Vietnamese/Asian fusion) — Ładna 1A. Mon–Sat 10:00–20:00. Vegan: Yes. Small venue. ∼15 min walk.
22. **Gluten Appetit** (Polish home–style) — Szczytnicka 54/1b. Mon–Fri 11:00–20:00, Sat-Sun 12:00-19:00. Vegan: No. Medium-sized venue. ∼10 min walk.
23. **Hi from India** (Indian) — Szczytnicka 36a. Mon–Sun 11:00–21:00. Vegan: Yes. Medium-sized venue. ∼5 min walk.

At the bottom, you'll find a QR code linking to the highlighted restaurants on Google Maps.



OTHER USEFUL INFORMATION

Weather: In September, daytime temperatures range from 15 to 25°C, nighttime temperatures from 10 to 15°C, with occasional rain.
Currency Exchange: You can exchange currency at the Grunwaldzki Square (look for signs saying “kantor”); rates: 1 USD = 3.65 zł, 1 EUR = 4.25 zł.
For the official exchange rate, vist: `http://www.nbp.pl/kursy/kursya.html`
ATMs: Available at the entrance of the C-6 building and inside the Pasaz Grunwaldzki shopping mall.

Emergency Numbers (Free from any phone)

- Ambulance / Medical Emergency: 999
- Fire: 998
- Police: 997
- General Emergency (mobile phones): 112

MDMM Emergency Contact

For any urgent matter during the conference, please contact:

- **Email:** mdmm@pwr.edu.pl

SIGHTSEEING CRUISE

The sightseeing cruise is planned for Wednesday, after the conference talks. Participants will have the opportunity to see the city of Wrocław from the perspective of a river boat and take a guided tour.

The first part, the Odra River Cruise, will start at the Szczytnicka Marina, located near the H-14 building (A). The cruise will start at 15:00 and will last approximately 1.5 hours.

After that, participants may disembark at the first stop, ZOO Marina (B), and begin a guided sightseeing tour of the Centennial Hall the Wrocław Fountain and the Pergola, **or** continue to the second stop, Dunikowskiego Marina (C), and begin a guided tour around Wrocław City Centre during which participants will see the Wrocław University, the Ossolineum and the Main Square. Both tours will be guided and will last approximately 1.5 hours.

Transport to the Banquet venue

From the Centennial Hall (each route takes approx. 40 minutes):

Route 1: 🚋 Tram 10 from ZOO (a) or Hala Stulecia (b) → Rynek (c) → 🚶 10 min walk to *La Maddalena* (D).

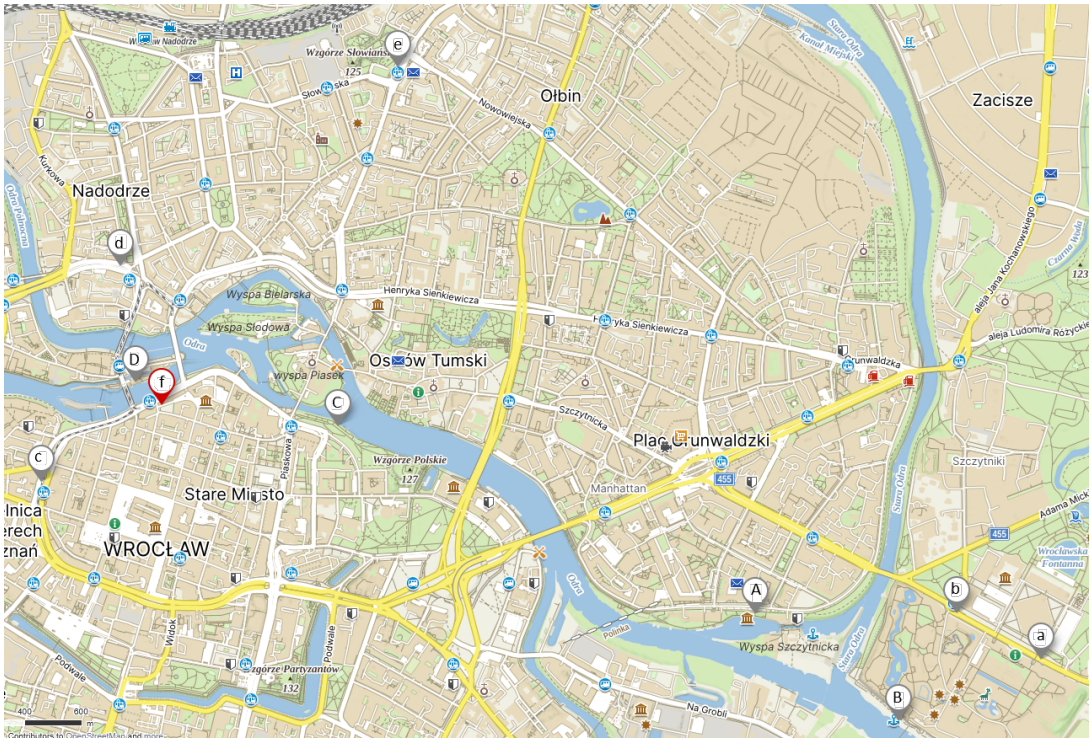
Route 2: 🚋 Tram 19 from ZOO (a) or Hala Stulecia (b) → Pomorska (d) → 🚶 9 min walk to *La Maddalena* (D).

Route 3: 🚋 Tram 1 from ZOO (a) or Hala Stulecia (b) → Nowowiejska (e), change here to 🚋 Tram 6 → Uniwersytet Wrocławski (f) → 🚶 4 min walk to *La Maddalena* (D).

The trams run frequently — Tram 10, 19, and 1 depart approximately every 5 minutes — so the waiting time will be short.

From Wrocław City Centre: *La Maddalena* restaurant is within a 🚶 20 minute walk from City Centre, so no public transport is suggested.

Note: For a self-guided cruise, we recommend using the *jakdojade* app (Web/iOS/Android) to plan 🚋 public transport routes, and the *Google Maps* for 🚶 walking or 🚗 driving directions in Wrocław.



CONFERENCE PROGRAM

September 7, 2025 (Sunday)

14:00- 18:00 Registration: Wyb. Wyspiańskiego 40, Building H-14a

September 8, 2025 (Monday)

9:00–9:15 Opening ceremony

Session I Applications of machine learning (Chair: K. Szalewicz)

9:15- 9:55 **B. Grzybowski** (Ulsan National Institute of Science and Technology, South Korea) *Algorithms for synthesis planning, reaction discovery and chemical industry*

9:55-10:25 **P. Dral** (Xiamen Univ., China; Nicolaus Copernicus Univ. in Toruń, Poland) *AI for learning across chemical space and quantum chemical methods*

10:25-11.05 Coffee break

Session II Modeling reactions & catalysts (Chair: B. Lesyng)

11:05-11:30 **U. Ryde** (Lund Univ., Sweden) *Computational studies of nitrogenase*

11.30-11:55 **V. Moliner** (Univ. Jaume I, Spain) *Towards the computational-assisted (re)-design of new enzymes for the recycling of synthetic polymers*

11:55-12:20 **A. Michalak** (Jagiellonian Univ., Poland) *Theoretical study on mechanisms of degradation of polymeric materials for fuel-cell applications*

12:20-12:40 P. Paneth (Łódź Univ. of Technology, Poland) *Mechanism of dehalogenation by F430*

12:40-13:00 Z. Wojdyła (J. Heyrovský Institute of Physical Chemistry, Czech Republic) *The variability of redox versus acid-base properties of tyrosine in an enzyme environment*

13:00-15.00 Lunch break

Session III Graduate student presentations (Chair: J. Korchowiec)

15:00-15.10 A. M. Tedy (Indian Institute of Technology Tirupati, India) *Role of naphthalene-to-azulene reconstruction in enhancing triplet photosensitization in chalcogenated biazulenediimides and reconstructed perylenediimides*

15.10-15.20 K. Szupryczyński (Collegium Medicum, Nicolaus Copernicus Univ. in Toruń, Poland) *Nedaplatin binding preferences: Vitamins from B group vs. nucleobases*

15.20-15.30 K. Baran (Gdańsk Univ. of Technology, Poland) *Few-shot machine learning modeling of sorption in ionic liquids*

15.30-15.40 Y. Didovets (Jagiellonian Univ., Poland) *The study of the interaction network between polymer chains in shape memory polyurethane copolymers*

15.40-15.50 J. Salekhe (Wrocław Univ. of Science and Technology, Poland) *TD-DFT Study of Photophysical Behavior and Charge Separation in Pincer Complexes for CO_2 Reduction*

15.50-16.00 D. Nowak (Adam Mickiewicz Univ. in Poznań, Poland) *Machine learning in drug discovery: Transforming medicinal chemistry through predictive modeling and innovative applications*

Session IV Poster session

16:15- 19:00 Poster presentation & coffee break

September 9, 2025 (Tuesday)

Session V Modeling Molecular Materials (Chair: A. Michalak)

9:00- 9:25 **M. Tuckerman** (New York Univ., USA) *Crystal Math: Rapid and accurate prediction of molecular crystal structures and properties using topological and simple physical descriptors, informatics, and machine learning models*

9:25- 9:50 **H. Ågren** (Wrocław Univ. of Science and Technology, Poland; Uppsala Univ., Sweden) *Nanoparticle plasmonics in the 1–10 nm ultrafine regime*

9:50-10:15 **T. Dornheim** (Helmholtz-Zentrum Dresden-Rossendorf, Germany) *Ab initio path integral Monte Carlo simulation of warm dense matter*

10:15-10:40 **J. Rak** (Univ. of Gdańsk, Poland) *Radiosensitizing nucleosides. Experimental and theoretical studies*

10.40-11.00 L. Chomicz-Mańka (Univ. of Gdańsk, Poland) *Oxygen mimetic or radioprotector suppressor: what is the role of metronidazole in radiosensitization*

11:00-11.30 Coffee break

Session VI Modeling Biomolecules & Drug Design (Chair: J. Rak)

11:30-11:55 **J. Grembecka** (Univ. of Michigan, USA) *Structure-based design of new therapeutics for leukemia: from bench to bedside and back*

11:55-12:20 **T. Cierpicki** (Univ. of Michigan, USA) *Challenges in development of small molecule inhibitors for difficult targets*

12:20-12:45 **J. Burda** (Charles Univ., Czech Republic) *Interactions of gold(I)-NHC complexes with models of Thioredoxin reductase; DFT & QM/MM studies*

12:45:13:05 N. Gresh (LCT UMR7616 CNRS Sorbonne Univ., France) *Sequence-selective targeting of the major groove of B DNA by oligopeptide conjugates of anthraquinone and cationic porphyrins*

13:05-15:00 Lunch break

Session VII Applications of machine learning (Chair: B. Grzybowski)

15:00-15.25 **K. Szalewicz** (Univ. of Delaware, USA) *New life for "classical" force fields in the age of machine learning*

15.25-15.50 **O. Isayev** (Carnegie Mellon Univ., USA) *AIMNet2: Foundation neural network potential for molecules and chemical reactions*

15.50-16:10 M. Hoffmann (Adam Mickiewicz Univ. in Poznan, Poland) *Artificial intelligence in chemistry: How to propose molecules with desired properties?*

16.10-16.30 B. Lesyng (Univ. of Warsaw, Poland) *Is the Development of Molecular Modeling Methods Subject to Evolutionary Laws?*

16.30-16.50 R. Szabla (Wrocław Univ. of Science and Technology, Poland) *Shedding UV light on DNA and RNA charge transfer*

16.50-17.10 P. Żuchowski (Nicolaus Copernicus Univ. in Toruń, Poland) *SAPT-Inspired Theory with Infinite-order Induction*

17:10-17.40 Coffee break

17:40-17:50 Conference photo

Session VIII Applications of AI & ML

17:50- 19:20 Panel discussion featuring the following Panelists:

P. Dral (Xiamen Univ., China, Nicolaus Copernicus Univ. in Toruń, Poland)

B. Grzybowski (Ulsan National Institute of Science and Technology, South Korea)

O. Isayev (Carnegie Mellon Univ., USA)

T. Kajdanowicz (Wrocław Univ. of Science and Technology, Poland)

T. Martinez (Stanford Univ., USA)

K. Szalewicz (Univ. of Delaware, USA)

September 10, 2025 (Wednesday)

Session IX Advances in computational methods (Chair: A. Eilmes)

9.00- 9.25 **T. Martinez** (Stanford Univ., USA) *Discovering Chemistry and Photochemistry from First Principles*

9.25- 9.50 **P. Piecuch** (Michigan State Univ., USA) *H_3 formation from methyl halogens and pseudohalogens: Experiment, theory, and governing factors*

9.50-10.15 **P. Imhof** (Friedrich Alexander Univ. Erlangen-Nurnberg, Germany) *Dissecting the effect of intra- and intermolecular interactions on conformational dynamics*

10.15-10.40 **T. Wesołowski** (Univ. of Geneva, Switzerland) *Extending the domain of applicability of Frozen-Density Embedding Theory based methods to chromophore-to-solvent charge transfer excitations*

10.40-11.00 A. J. Kałka (Jagiellonian Univ., Poland) *Electrostatic embedding QM/MM approach for exploration of enzyme activity — trust, but verify*

11:00-11.30 Coffee break

Session X Modeling Molecular Materials (Chair: T. Wesołowski)

11.30-11.55 **A. Eilmes** (Jagiellonian Univ., Poland) *Interactions in solutions studied via vibrational spectra from molecular dynamics simulations*

11.55-12:20 **J. Korchowiec** (Jagiellonian Univ., Poland) *Indirect Constructions for Improving the Accuracy of Fragmentation Methods*

12.20-12.40 H. Dominguez (Universidad Nacional Autónoma de México, Mexico) *Use of synthetic and biosurfactant molecules as contaminant removal agents in solid and aqueous media*

12.40-13.00 Y. Bushuev (Univ. of Silesia in Katowice, Poland) *Modeling of micro/nanorockets propulsion based on fast water expulsion from hydrophobic nanoporous materials*

13.00-15.00 Lunch break

15:00-18.00 Excursion

19.00-21.00 Conference banquet

September 11, 2025 (Thursday)

Session XI Modeling Molecular Materials (Chair P. Piecuch)

9.00- 9.20 P. Cysewski (Collegium Medicum, Nicolaus Copernicus Univ. in Toruń, Poland) *Computational Approaches for Designing Effective and Pharmaceutically Acceptable Solvents for Active Pharmaceutical Ingredients*

9.20- 9.40 P. Dopieralski (Univ. of Wrocław, Poland) *Mechanochemical disulfide reduction – computational study*

9.40-10.00 A. Spyszkiewicz (Wrocław Univ. of Science and Technology, Poland) *Kinetic modeling of prebiotic networks activated by methyl isonitrile*

10.00-10.20 F. Šebesta (J. Heyrovský Institute of Physical Chemistry, Czech Republic) *Hole hopping via artificial Trp pathways in azurin mutants*

10.20-10.40 A. Jezuita (Jan Długosz Univ. of Częstochowa, Poland) *Substituent effects on the electron transfer mechanism in dye–ZnO photovoltaic systems: a quantum chemical analysis*

10.40-11.15 Coffee break

Session XII Modeling Molecular Materials (Chair: J. Burda)

11.15-11:35 A. Stachowicz-Kuśnierz (Jagiellonian Univ., Poland) *Interactions of ultra-fine polystyrene nanoparticles with lung surfactant monolayers and bilayers*

11.35-11:55 M. Makowska-Janusik (Jan Długosz Univ. of Częstochowa, Poland) *The adsorption of Ru-based dyes on the surface of the TiO_2 anode to enhance the photovoltaic efficiency of DSSC devices — computational approach*

11.55-12.15 K. Hęclik (Rzeszów Univ. of Technology, Poland) *Study of intermolecular interactions of polymer compositions based on P3HB*

12.15-12.35 P. Ordon (Wrocław Univ. of Life and Environmental Sciences, Poland) *Chemical reactivity derived from molecular forces*

12:35-12.50 Conference closing

Note: Invited speakers are indicated in **bold**.

MDMM2025 CONFERENCE POSTERS

Poster No.	Presenting Author	*Poster Title*
1	Johnrich Attupuram Joychan	*DFT Investigation of MXene–based Nanomaterials for Methanol Oxidation Reaction in Direct Methanol Fuel Cells (DMFCs)*
2	Karol Baran	*Few-shot Machine Learning Modeling of Sorption in Ionic Liquids*
3	Andrzej Bil	*The Dissociation of Macrocyclic Disulfide Complexes — Topological Study*
4	Yuxinxin Chen	*UAIQM — the Ultimate Solution to the Universal AI Models for Atomistic Simulations Beyond DFT*
5	Sylwia Czach	*Understanding Mechanistic Transitions in Photoactive Yellow Protein with Machine Learning*
6	Yuliia Didovets	*The Study of the Interaction Network between Polymer Chains in Shape Memory Polyurethane Copolymers*
7	Edyta Dyguda-Kazimierowicz	*Evaluating Drug Resistance-Related Mutations via First-Principles Interaction Energy Analysis*
8	Tomáš Grycz	*Hole Hopping Between an Oxidized Tryptophan and the Cu(I) Centre in Azurin Constructs. QM/MM Study.*
9	Mikołaj Gurba	*Base Stacking Interactions and Photoinduced Electron Transfer in Nucleic Acids*
10	Maciej Hapke	*Mechanistic Insight into Stereoselectivity of Beta vulgaris 4,5-Extradiol Dioxygenase*
11	Yifan Hou	*Making Expensive Simulations Affordable: AI for IR and Raman*
12	Mateusz Jędrzejewski	*Atomic Population: the Inherent Parameter for and Atom-in-Molecule Calculated Analytically from the Electron Density Function*
13	Mercedes Kukułka	*Theoretical Insights into the Stability of Carbazolium Cations for Alkaline Fuel Cell Membranes*
14	Barbara Lech	*Mechanistic Studies of DNA Nonenzymatic Primer Extension*
15	Samanta Makurat	*Computational Insights into Human Lysosomal α-Glucosidase: Advancing Pompe Disease Research*
16	Łukasz Mioduszewski	*Predicting Structure and Properties of Polytryptophan Crystals*
17	Tymoteusz Mrozek	*Calculations of High Accuracy Dynamic Polarizabilites of Excited States by Means of ECG Basis Set*
18	Hassan Nawaz	*Aitomia: Your Intelligent Assistant for AI-Driven Atomistic and Quantum Chemical Simulations*
19	Damian Nowak	*Machine Learning in Drug Discovery: Transforming Medicinal Chemistry through Predictive Modeling and Innovative Applications*
20	Boluwatife Ogunnaiya	*Computational Investigation of the Effect of Mg^2 Cations on Nonenzymatic Self-Replication of RNA*
21	Michał Pocheć	*Machine Learning in Studies of RNA Nucleosides Conformations*
22	Maria Rózga	*Theoretical Study on the Decomposition of Isoindolinium Cations in Alkaline Fuel Cells*
23	Marwa Saad	*Investigation of PVC and Plasticizers Present in Heritage Collection by Theoretical Calculations*

24	Filip Sagan	*Theoretical Characterization of Melanin Degradation Products: Intermolecular Interactions and Triplet State Energetics*
25	Ana Beatriz Salazar-Arriaga	*Instability of Ionic Surfactants Monolayers at the Water/Air Interface Induced by Biosurfactants: A Molecular Dynamics Investigation*
26	Jabir Salekhe	*TD-DFT Study of Photophysical Behavior and Charge Separation in Pincer Complexes for CO_2 Reduction*
27	Saruti Sirimatayanant	*Investigating the Effects of the Immediate Environment of Rhodopsin on its 2PA Signal with QM/MM*
28	Maciej Spiegel	*In Silico Design of Anthraquinone Derivatives as Effective Two-Photon Photosensitizers for Photodynamic Therapy*
29	Rafał Stottko	*RGBChem: Image-like Representation of Chemical Compounds for Properties Prediction*
30	Maksymilian Szatko	*Solvent Dependent Helical Folding of Sequence-Defined Oligourethanes*
31	Adrian Szczyrba	*The Influence of Hydration Level on Dissociative Electron Attachment to 1,3-Dimethyl-5-Thiocyanatouracil — Computational and Experimental Studies*
32	Kamil Szupryczyński	*Nedaplatin Binding Preferences: Vitamins from B group vs. Nucleobases*
33	Paweł Śliwa	*Fragment Molecular Orbital Method as a Tool for Studying G Protein-Coupled Receptors*
34	Annette Mariya Tedy	*Role of Naphthalene-to-Azulene Reconstruction in Enhancing Triplet Photosensitization in Chalcogenated Biazulenediimides and Reconstructed Perylenediimides*
35	Kasper Witruk	*From Torsion Angles to Folding Pathways: Data-Driven Analysis of Oligourethane Dynamics*
36	Franciszek Włodek	*Exploration of Oxidation of Lipids in Lung Surfactant Model*
37	Jarosław Zaklika	*Local and Global Electronic Softness of Linear Molecules*
38	Jarosław Zaklika	*Analytic Approach to the Local and Global Softness in Atoms and Their Ions*
39	Olga Żurowska	*Application of Differential Molecular Electrostatic Potential (ΔMEP) in a Description of Chemical Bonding and Reactivity*