



Warsaw-4-PhD
Warsaw Doctoral School
in Natural and Biomedical Sciences



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IChF

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Warsaw Doctoral School in Natural and Biomedical Sciences and the Institute of Physical Chemistry PAS cordially invites you to an **ADVANCED LECTURE SERIES – BIOLOGY-INSPIRED CHEMISTRY** talk.

Photoinduced functionality of molecular assemblies modulated by their dynamics in a material

given by

dr. Mariana Kozłowska

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on 12th December 2024, 10:00 at IChF Aula
Duration: 60 min + question time

Highly recommended to all Warsaw-4-Phd students!

An interesting concept, permitting the study of a variety of new photophysical phenomena is based on the assembly of modulated light- and electron-responsive materials. Three-dimensional structure of such materials is often driven by noncovalent interactions that control intermolecular interaction patterns and condensed state geometries.^[1,2] However, the resultant optoelectronic response may also be significantly impacted by the vibrational flexibility of molecules in an assembly. The prediction of noncovalent interactions, the control of supramolecular assembly and the consideration of materials' dynamics are challenging, limiting further modification of molecules for new materials with desired photoinduced properties.

In my talk, I will demonstrate the application of multiscale modeling and automated workflow tools for understanding the assembly of functional organic molecules in pillar-layered and surface-anchored metal-organic frameworks.^[3,4] I will explain the prediction of their photoconductive, photoswitchable and chiroptical properties, as well as the molecular bases of light-induced phenomena and the influence of noncovalent interactions and molecular motions.
[1,4,5]

References

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- [2] Haldar, R.; Jakoby, M.; Kozłowska, M.; Khan, M.R.; Chen, H.; Pramudya, Y.; Richards, B.S.; Heinke, L.; Wenzel, W.; Odobel, F.; Diring, S.; Howard, I.A.; Lemmer, U.; Wöll, C., *Chem. Eur. J.* **2020**, *26*, 17016-17020.
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- [5] Li, C.; Schopmans, H.; Langer, L.; Marschner, S.; Chandresh, A.; Bürck, J.; Tsuchiya, Y.; Chihaya, A.; Wenzel, W.; Bräse, S.; Kozłowska, M.; Heinke, L., *Angew. Chem. Int. Ed.*, **2023**, *62* (10), e202217377.

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