Session number, lecture date and time (to be filled by the organizer)

DYNAMIC CRYSTALS – A NEW CLASS OF SMART ENGINEERING MATERIALS

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Abstract:
The anticipated shift in focal point of interest of solid- state chemists, crystal engineers and crystallographers from structure to properties to function of organic solids parallels the need to apply our accumulated understanding of the intricacies of crystal structure to explaining the related properties, with the ultimate goal of harnessing that knowledge in applications that require soft, light-weight, and/or biocompatible organic solids. In these developments, the adaptive molecular single crystals warrant a particular attention as a new class of materials for light, flexible, and environmentally benign devices, primarily memories, capacitors, sensors, and actuators. Some of the outstanding requirements for application of these dynamic materials as high-efficiency energy storage devices are strongly induced polarization, high switching field, and narrow hysteresis in reversible dynamic processes. However, having been studied almost exclusively by crystallographers, molecular crystals still lack the appropriate investigations that reliably evaluate their reproducibility, scalability, and actuating performance, and some important drawbacks have diverted the interest of engineers from these materials. United under the umbrella term crystal adaptronics, the recent research efforts aim to realistically assess the appositeness of dynamic crystals for applications that require fast, reversible and continuous operation over prolonged periods of time. With the aim to highlight the most recent developments in the research of adaptive molecular crystals, this lecture discusses their assets and pitfalls. Using machine learning for the first time, we identify inherent features and structure-function relationships that fundamentally impact the mechanical response of dynamic molecular crystals. Our approach factors in different crystal properties in tandem and deciphers their intersectional and combined effects on the dynamic performance. It also provides some hints on the likely future developments that capitalize on the untapped, sequestered potential for applications of this distinct materials class.

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Biography:

Panče Naumov holds the position of full professor of chemistry with tenure at New York University Abu Dhabi (NYUAD). He also serves as a Global Network Professor of Chemistry at New York University's Faculty of Arts and Sciences and holds a cross-appointment at New York University's Molecular Design Institute. Additionally, he acts as the Director of the NYUAD Center for Smart Engineering Materials (CSEM), and leads the Smart Materials Lab (SML) at NYUAD. Naumov's Smart Materials Lab is widely recognized as the leading research team in chemistry and materials science in the UAE. According to Nature Index, the lab's output accounts for approximately 40-60 percent of both the number and fractional count of the high-impact publications in chemistry in the country each year. Furthermore, Naumov has been a fellow of the Radcliffe Institute at Harvard University.

Naumov obtained his PhD in chemistry and materials science from the Tokyo Institute of Technology in 2004, complemented by a BSc from Ss Cyril & Methodius University in Macedonia. Prior to joining NYU Abu Dhabi and NYU, he held research fellow positions at the Japanese National Institute for Materials Science (NIMS) and faculty roles at Osaka University and Kyoto University in Japan. With a research portfolio comprising approximately 300 publications, Naumov's group has secured over USD 15 million in extramural funds, along with substantial start-up and internal funding over the last two decades. He has delivered approximately 400 presentations at conferences and scientific gatherings, including over 90 invited talks at various institutions. Since 2012, he has mentored more than 60 students, overseeing PhD theses, undergraduate projects, and Capstone projects. Naumov is an active reviewer for around 100 international journals and over ten national and international funding agencies.

Naumov serves as a member of the editorial or advisory boards for several reputable journals, such as Angewandte Chemie, Chemistry - A European Journal, Chemistry - an Asian Journal, Smart Molecules, SmartMat, FlexMat, Wearable Electronics, and ChemNanoMat. Furthermore, he has contributed as a guest editor for the Proceedings of the National Academy of Sciences of the USA and currently holds the position of Associate Editor for the Journal of the American Chemical Society (JACS), overseeing solid-state chemistry, photochemistry, crystallography, and crystal engineering.

Representative Publications:

[1] Mahmoud Halabi, J., Al-Handawi, M. B., Ceballos, R., Naumov, P. (2023) J. Am. Chem. Soc. 145, 12173.

[2] Awad, W. M., Davies, D. W., Kitagawa, D., Mahmoud Halabi, J., Al-Handawi, M. B., Tahir, I., Tong, F., Campillo-Alvarado, G., Shtukenberg, A. G., Alkhidir, T., Hagiwara, Y., Almehairbi, M., Lan, L., Hasebe, S., Prasad Karothu, D., Mohamed, S., Koshima, H., Kobatake, S., Diao, Y., Chandrasekar, R., Zhang, H., Sun, C. C., Bardeen, C., Al-Kaysi, R. O., Kahr, B., Naumov, P. (2023) Chem. Soc. Rev. 52, 3098.
[3] Karothu, D. P., Mahmoud Halabi, J., Ahmed, E., Ferreira, R., Spackman, P. R., Spackman, M. A., Naumov, P. (2022) Angew. Chem. Int. Ed. 61, e202113988.
[4] Spackman, P. R., Grosjean, A., Thomas, S. P., Karothu, D. P., Naumov, P., Spackman, M. A. (2022) Angew. Chem. Int. Ed. 134, e202110716.
[5] Mahmoud Halabi, J., Ahmed, E., Sofela, S., Naumov, P. (2021) Proc. Nat. Acad. Sci. USA 118, e2020604118.
[6] Naumov, P., Karothu, D. P., Ahmed, E., Catalano, L., Commins, P., Mahmoud Halabi, J., Al-Handawi, M. B., Li, L. (2020) J. Am. Chem. Soc. 142, 13256.
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