**Five-Day National Workshop on Molecular Dynamics Simulation and Analysis Concludes at NIT Jalandhar**

The Department of Mechanical Engineering, Dr. B R Ambedkar National Institute of Technology (NIT) Jalandhar, successfully organized a **five-day national workshop on "Molecular Dynamics Simulation and Analysis"** from **28th July to 1st August 2025**. The event brought together leading experts and enthusiastic participants from across the country to delve into the fundamentals and advanced applications of molecular dynamics (MD) simulations in materials research and engineering.

The workshop featured expert lectures and hands-on training sessions delivered by a distinguished panel of speakers, including:

- **Prof. S. P. Singh**, Indian Institute of Technology (IIT) Delhi
- **Prof. Navin Kumar**, IIT Ropar
- **Prof. Tamal Banerjee**, IIT Guwahati
- **Prof. Shailesh Kundalwal**, IIT Indore
- **Prof. Shahram Ajori**, University of Maragheh, Iran
- **Dr. Sumit Sharma**, NIT Jalandhar

The workshop was coordinated by **Dr. Sumit Sharma** and **Dr. Ashok Kumar**, both Assistant Professors in the Department of Mechanical Engineering at NIT Jalandhar. Their efforts ensured a well-structured and engaging academic event, emphasizing the practical learning experience for the participants.

The inauguration ceremony was graced by **Prof. B. K. Kanaujia**, Director, NIT Jalandhar, who highlighted the growing significance of computational tools like molecular dynamics in solving complex engineering problems. **Prof. Rohit Mehra**, Dean (Research & Consultancy), **Prof. T Srinivas**, Head (Mechanical Engineering), and **Prof. Arvind Bhardwaj**, Head (Centre for Continuing Education), also addressed the gathering, emphasizing interdisciplinary collaboration and the importance of skill-based training for research scholars and faculty. Molecular Dynamics (MD) simulation has emerged as a powerful computational technique to study the behavior of materials at the atomic and molecular scale. It enables researchers to predict mechanical, thermal, and transport properties, investigate failure mechanisms, and design new materials for advanced engineering applications. With its increasing relevance across disciplines like materials science, physics, chemistry, and bioengineering, MD is now a critical tool for both academic research and industrial innovation.

Over 25 participants from prestigious institutes such as **IIT Dharwad, IIT Mandi, NIT Hamirpur, NIT Calicut, NIT Rourkela, IGCAR Kalpakkam**, and other reputed academic and research organizations took part in the workshop. A key highlight of the event was the **hands-on training on open-source molecular dynamics software LAMMPS**, where participants explored the simulation of nanostructures, polymers, and crystalline materials under expert guidance.

The workshop concluded with a valedictory session acknowledging the enthusiastic participation, knowledge-sharing, and future research collaborations inspired by the event.