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Dept. of Applied Chemistry (DAC), CUSAT

"Artificial Intelligence for Chemistry"

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COCHIN UNIVERSITY OF SCIENCE AND TECHNOLOGY

Venue: Seminar Hall, DAC, CUSAT

Artificial Intelligence for Chemistry

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Modern machine learning methods have had phenomenal success in the technology areas such as computer vision, speech recognition, natural language processing (NLP), etc. Inspired by this, we see a surge in the use of artificial intelligence-machine learning methods to address problems in fundamental sciences during the last few years. Availability of high performance Graphics Processing Unit (GPU) accelerators, large datasets, novel algorithms, and libraries have positively contributed to enhanced activity in this area. In chemistry, ML methods have been successfully applied to various problems such as predicting accurate energies of molecules, various drug discovery tasks, retrosynthetic pathway prediction, inverse design of molecules, etc. This talk will discuss the impact AI methods in general have made in chemistry research and gives a conceptual overview of different ML methods. Recent efforts of using artificial neural networks, convolutional neural networks, reinforcement learning and Monte Carlo tree search for carrying out various prediction/classification tasks in molecular design, molecular generation, and prediction of molecules starting from their spectra will be discussed.