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Computers in Chemistry

Harnessing the Power of AI/ML in Molecular Design and Discovery

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Date: **Friday, March 31, 2023**
Register here
(or Scan QR Code)

Time: 11:00 AM EDT via Zoom

Abstract
The efficient design of target-or organism-driven molecules is a crucial aspect of therapeutic discovery and biological mechanism. However, traditional approaches often suffer from slow iterative design-test cycles and are heavily dependent on the expertise of the scientists, resulting in bottlenecks in molecular design. In this talk, I will discuss the transformative potential of foundational artificial intelligence (AI) and machine learning (ML) by leveraging physics based modeling and simulations, large scale workflow, advanced algorithms, and active feedback loop. Deep reinforcement learning (RL) provides an efficient way to optimize key features by a multi-objective reward function within a protein pocket using parallel graph neural network models. The agent learns to build molecules in 3D space using generative adversarial networks while optimizing key biophysical properties targeted towards a specific protein target. Our approach can serve as an interpretable AI tool for lead optimization with optimized activity, potency, and biophysical properties

Biography
Dr. Neeraj Kumar is a data scientist and program development lead at Pacific Northwest National Laboratory. His scientific contributions and publication profile cover a range of topics on applied machine learning, deep learning, probabilistic programing, natural language processing, quantum computing, and simulations methods for applied and fundamental science application. He and his team are working on the development of physics and bio-informed machine learning models to build autonomous decision making tools to address the challenges associated with unstructured complex heterogeneous data. He has been developing new research direction, leading technical programs and driving scalable AI/ML products with focus on modeling, cloud computing, and advanced analytical methods to address fundamental scientific questions in computational chemistry and biology (digital molecular discovery).