

# **AIMNet2: Foundation neural network potential for molecules, reactions, and CADD-related tasks**

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Deep learning is revolutionizing many areas of science and technology, particularly in natural language processing, speech recognition, and computer vision. In this talk, we will provide an overview of the latest developments in machine learning and AI methods and applications to the problem of drug discovery and molecular design at Isayev's Lab at CMU. We identify several areas where existing methods have the potential to accelerate computational chemistry research and disrupt more traditional approaches.

Machine-learning interatomic potentials (MLIPs) are reshaping computational chemistry practices because of their ability to drastically overcome the accuracy-length/time-scale trade-off. In this work, we present the 2nd generation of our atoms-in-molecules neural network potential (AIMNet2), which is applicable to species composed of up to 14 chemical elements in both neutral and charged states, making it a valuable model for modeling the majority of non-metallic compounds. AIMNet2 combines ML-parameterized short-range and physics-based long-range terms to attain generalizability that ranges from simple organics, reaction, and crystal structures to diverse molecules with "exotic" element-organic bonding.