Contribution ID: **21** Type: **Oral talk**

A neural network model of the dependence of the energy of biomolecules on structure and quantum-mechanical descriptors

Thursday, 12 June 2025 14:40 (20 minutes)

The development of new molecules and the optimization of chemical synthesis depend on the ability to accurately estimate molecular energies and properties from structural information. In recent years, machine learning (ML) methods have emerged as powerful tools for addressing this task [1]. However, a persistent challenge is the illusion of improved accuracy that arises due to error compensation effects. This issue occurs when a ML model attempts to approximate the total energy directly, rather than modeling its individual physical components separately. By directly approximating the total energy, such models may rely on error compensation between components, which masks inaccuracies and undermines generalization to new molecular systems.

To address these challenges, we leverage principles from density functional theory (DFT) and graph neural networks (GNNs). Our approach aims to explore the feasibility of constructing a neural network model for predicting total molecular energy through a two-stage process. In the first stage, physically motivated descriptors are generated based on electron density and kinetic energy contributions, which are associated with individual atoms or atom pairs rather than the molecule as a whole. In the second stage, these descriptors are used to approximate the parameters of a classical interatomic potential using a separate neural network.

We demonstrate the effectiveness of our approach on publicly available datasets by accurately predicting both the total molecular energy and the electronic kinetic energy, with a mean absolute error (MAE) of 2.2 kcal/mol and 6.1 kcal/mol, respectively. Additionally, the model yields reliable results in the task of estimating intermolecular interaction energies, achieving a mean squared error (MSE) of 1.7 kcal/mol.

1. Sajjan M., Li J., Selvarajan R., Sureshbabu S.H., Kale S.S., Gupta R., Singh V., Kais S. Quantum machine learning for chemistry and physics // Chem. Soc. Rev. – 2022. – 51(15). – P. 6475–6573. – DOI: 10.1039/D2CS00203E.

Primary authors: TERETS, Andrii (Faculty of Physics of Taras Shevchenko National University of Kyiv); NIKOLAIENKO, Tymofii (Taras Shevchenko National University of Kyiv)

Presenter: TERETS, Andrii (Faculty of Physics of Taras Shevchenko National University of Kyiv)

Session Classification: Artificial Intelligence in Physics

Track Classification: Artificial Intelligence in Physics