Showcasing research from the laboratories of Professors Brett M. Savoie and Olexandr Isayev, School of Chemical Engineering at Purdue University and School of Chemistry at Carnegie Mellon University, respectively.

Δ^2 machine learning for reaction property prediction

Reaction properties derived from high-level transition state calculations are prohibitively expensive to predict in many scenarios. The current works shows that machine learning models can be trained to learn high-level transition state properties from approximate geometries calculated at a lower level of theory. The general approach is referred to as Δ^2 machine learning because the models learn differences in both geometry and energy between the low and high-level predictions. The approach can be extended to other critical points and is compatible with transfer learning to different levels of theory.

As featured in:

See Olexandr Isayev, Brett M. Savoie *et al.*, *Chem. Sci.*, 2023, **14**, 13392.

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