Machine Learning Approaches for Efficient and Accurate Reaction Network Analysis

Tutorial and Training Material

Modeling Potential Energy Functions with Machine Learning and Classical Techniques

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Hands-on Session

Accurately predicting reaction barrier heights associated with transition state (TS) structures is essential for understanding chemical reactivity in areas such as combustion chemistry, catalysis, and reaction network modeling. Although high-level electronic structure methods provide reliable results, their computational cost becomes prohibitive when dealing with large reaction datasets.

In this hands-on session, we explore how modern **machine learning approaches**, and in particular the **MACE architecture**,[1,2] can be used to efficiently learn potential energy surfaces and predict **barrier heights (BHs)** and **reaction enthalpies (REs)** with high accuracy.

We will work with a curated dataset of gas-phase organic reactions including reactants, transition states, and products computed at the DFT level.[3] First, participants will train **direct learning models** that predict DFT energies from molecular structures. Subsequently, a Δ-learning strategy will be introduced, where MACE is trained to learn systematic energy corrections to a fast semiempirical baseline (GFN2-xTB[4]), significantly improving accuracy even with limited training data.

Throughout the session, participants will:

- Build and organize reaction datasets.
- Visualize reaction pathways and transition states in 3D.
- Train MACE ML models using both direct learning and Δ-learning approaches.
- Evaluate model performance for energies, barrier heights, and reaction enthalpies.

This session highlights how machine learning can bridge the gap between accuracy and efficiency, enabling scalable prediction of reaction barriers and providing a foundation for future developments toward direct transition state prediction.

To access the session materials, scan the QR code below or use the link:

https://github.com/OmarRodriguezLopez1398/ML_Corrections_Reactions_Training

References

[1] Batatia, I.; Kovacs, D. P.; Simm, G. N. C.; Ortner, C.; Csanyi, G. MACE: Higher order equivariant message passing neural networks for fast and accurate force fields. Advances in Neural Information Processing Systems. 2022.

[2] Kovács, D. P.; Moore, J. H.; Browning, N. J.; Batatia, I.; Horton, J. T.; Pu, Y.; Kapil, V.; Witt, W. C.; Magdău, I.-B.; Cole, D. J.; Csányi, G. *J. Am. Chem. Soc.* **2025**, *147*, 17598–17611.

[3] Spiekermann, K.; Pattanaik, L.; Green, W. H. *Sci. Data* **2022**, *9*, 417.

[4] Bannwarth, C.; Ehlert, S.; Grimme, S. *J. Chem. Theory Comput.* **2019**, *15*, 1652–1671.