Session of "Fokus Materialchemie" – Wednesday, **21.01.2026** 14:00
@ Seminarraum BA 05 (TU-Wien, Getreidemarkt 9, BA, OG. 05, BA05G02)
join us on ZOOM (ID: 983 0066 2349)

Integrating Nudged Elastic Band with Flow Matching for Enhanced Transition State Prediction

S. Gstoettenmayr[1], L. Galustian[1], K. Mark[1], E. Heid[1]

stephanie.gstoettenmayr@tuwien.ac.at

[1]Institute of Materials Chemistry, TU Wien, Austria

Accurate transition state prediction determines the activation energy and reaction kinetics of chemical reactions. Knowing these allows us to understand reaction mechanisms and optimize conditions to favor desired products while avoiding unwanted side reactions. GoFlow is a tool for generating transition state geometries directly from 2D molecular reaction graphs using flow matching with E(3)-equivariant neural networks [1]. This work proposes integrating the Nudged Elastic Band (NEB) [2] method with the GoFlow framework to enhance transition state prediction accuracy. Incorporating NEB images as additional training data into the flow matching model provides a favorable initial guess for the pathway progressing from reactant to product. Intermediate geometric information along reaction pathways could improve the quality of transition state generation.

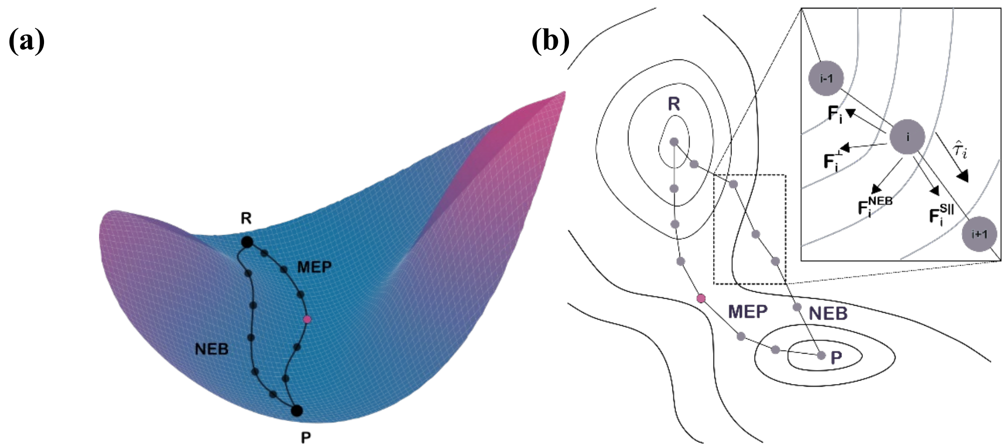

Illustration of the Nudged Elastic Band (NEB) method for finding Minimum Energy Paths (MEPs). (a) 3D plot of potential energy surface (PES) showing the NEB calculation converging to the MEP. The MEP represents the theoretical minimum energy pathway connecting reactant and product minima, passing through the transition state saddle point (colored in pink). The NEB images are geometric configurations connected by springs that iteratively optimize to approximate this MEP through force-based relaxation. (b) Contour plot with inset showing the NEB force projection scheme. The inset demonstrates how forces are decomposed: potential forces $F_i^{\perp}$ act perpendicular to the band to drive images toward the MEP, while spring forces $F_i^{S\|}$ act parallel to the band to maintain equal spacing between images.

[1] L. Galustian, K. Mark, J. Karwounopoulos, M. P.-P. Kovar, and E. Heid, 'GoFlow: Efficient Transition State Geometry Prediction with Flow Matching and E(3)-Equivariant Neural Networks', June 18, 2025, *Chemistry*. doi: 10.26434/chemrxiv-2025-bk2rh-v2.

[2] H. Jónsson, G. Mills, and K. W. Jacobsen, 'Nudged elastic band method for finding minimum energy paths of transitions', in *Classical and Quantum Dynamics in Condensed Phase Simulations*, LERICI, Villa Marigola: WORLD SCIENTIFIC, June 1998, pp. 385–404. doi: 10.1142/9789812839664_0016.