Ver. 17 May 2025

2025 "Computational Materials Chemistry" Telluride Workshop
Telluride Intermediate School, 725 W Colorado Ave, Telluride, CO 81435
Monday morning, 21 July 2025 to Friday noon, 25 July 2025; Breakfast starts 7:30am at School

Monday, 21 July 2025
8:00am-8:10am opening remarks
Session I: **Finding transition states**; Chairs: De-en Jiang/Bettina Keller
8:10am-9:00am Graeme Henkelman: From transition states to dynamics over long time scales
9:00am-9:50am Shin-ichi Koda: Alternative tools for double-ended transition state search
9:50am-10:20am Coffee Break
10:20am-11:10am Sam Blau: Neural Network Path Optimization for Finding Transition States on an MLP
11:10am-12:00pm Karsten Reuter: Automatic process exploration through ML assisted TS searches

Tuesday, 22 July 2025
Session II: **Machine learning**; Chairs: Greg Beran/Qing Zhao
8:10am-9:00am Zachary Ulissi: Machine learning potentials for everything (including transition state search)
9:00am-9:50am Johannes Margraf: ML-driven Reaction Network Exploration: Are we there yet?
9:50am-10:20am Coffee Break
10:20am-11:10am Jutta Rogal: Combining ML and Stat. Mech. to Accelerate Molecular Simulations
11:10am-12:00pm Lei Li: Charge-Optimized Atom-Centered NN Potential and Uncertainty Quantification

Wednesday, 23 July 2025
Session III: **Gen AI, beyond scaling, PES, and beyond TS**; Chairs: Mira Todorova/Shin-ichi Koda
8:10am-9:00am Mingjie Liu: Open Mat/Mol Generation: generative AI in chemistry
9:00am-9:50am C. Lawrence Zitnick: The limits of scaling and moving beyond computational models
9:50am-10:20am Coffee Break
10:20am-11:10am Lucas Bao: Bayesian Exploration and Construction of First-Principle PESs
11:10am-12:00pm Brett Savoie: More Transition States Than We Know What to Do With. What's Next?

Thursday, 24 July 2025
Session IV: **Interfaces**; Chairs: Joerg Neugebauer/Mingjie Liu
8:10am-9:00am Yuanyue Liu: Constant Potential Molecular Dynamics for Electrochemical Interface
9:00am-9:50am Christoph Scheurer: Modelling realistic interfaces in energy conversion materials
9:50am-10:20am Coffee Break
10:20am-11:10am Mira Todorova: Free energy surfaces for charge transfer reactions
11:10am-12:00pm Rob Wexler: Systematically Improvable Sampling of Interfacial Configuration Spaces

Friday, 25 July 2025
Session V: **Reaction, Catalysis, Solid State, and Phases**; Chairs: Graeme Henkelman/Karsten Reuter
8:10am-9:00am Bettina Keller: Thermal isomerization of retinal: from transition state theory to simulation
9:00am-9:50am Qing Zhao: Catalysis at Atomic Scale: Insights from Accurate Electronic Structure Theory
9:50am-10:20am Coffee Break
10:20am-11:10am Greg Beran: Predicting reactions in the organic solid state
11:10am-12:00pm Joerg Neugebauer: Computationally efficient automated computation of phases, phase transitions and diagrams

12:00pm – 12:15pm Concluding remarks; adjourn.