

2025 "Computational Materials Chemistry" Telluride Workshop

Samueli Room, Telluride Science and Innovation Center, 300 S Townsend St, Telluride, CO 81435

Monday morning, 21 July 2025 to Friday noon, 25 July 2025; Breakfast starts 7:30am at the venue

Sunday, 20 July 2025, 5:00pm to 6:30pm: cash-bar, Meet & Greet at Alibi – 157 S. Fir Street; badge pickup

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

2:00pm-2:50pm Zack Ulissi: Machine learning potentials for everything (including transition state search)

2:50pm-3:40pm Johannes Margraf: ML-driven Reaction Network Exploration: Are we there yet?

3:40pm-4:10pm Coffee Break

4:10pm-5pm Jutta Rogal: Combining ML and Stat. Mech. to Accelerate Molecular Simulations

5:00pm-5:40pm De-en Jiang: MLFFs for Amorphous Solid Electrolytes

5:40pm-6:00pm Ilgar Baghishov: Accuracy of the ML foundation models

Wednesday, 23 July 2025

Session III: **Gen AI, beyond scaling, PES, and beyond TS**; Chairs: Mira Todorova/Shin-ichi Koda

1:30pm-2:20pm Mingjie Liu: Open Mat/Mol Generation: generative AI in chemistry

2:20pm-3:10pm C. Lawrence Zitnick: The limits of scaling and moving beyond computational models

3:10pm-3:40pm Coffee Break

3:40pm-4:30pm Lucas Bao: Bayesian Exploration and Construction of First-Principle PESs

4:30pm-5:20pm Brett Savoie: More Transition States Than We Know What to Do With. What's Next?

5:30pm-8pm: Picnic, free and open to family/guests in the tent behind the Telluride Intermediate School.

Thursday, 24 July 2025

Session IV: **Interfaces and Catalysis**; Chairs: Joerg Neugebauer/Mingjie Liu

8:10am-9:00am Mira Todorova: Free energy surfaces for charge transfer reactions

9:00am-9:50am Christoph Scheurer: Modelling realistic interfaces in energy conversion materials

9:50am-10:20am Coffee Break

10:20am-11:10am Qing Zhao: Catalysis at Atomic Scale: Insights from Accurate Electronic Structure Theory

11:10am-11:35am Caitlin McCandler: Dynamical models for catalysis on featured surfaces

11:35am-12:00pm Alexandra Zagalskaya: Degradation and Catalytic Activity at Metal Oxide Interfaces

Friday, 25 July 2025

Session V: **Retinal Reaction, Solid State, Phases, and 2D**; Chairs: Karsten Reuter/Zachary Ulissi

8:10am-9:00am Bettina Keller: Thermal isomerization of retinal: from transition state theory to simulation

9:00am-10:50am Greg Beran: Predicting reactions in the organic solid state

9:50am-10:20am Coffee Break

10:20am-11:10am Joerg Neugebauer: Automated computation of phases, phase transitions and diagrams

11:10am-11:35am Konstantin Klyukin: mechanisms of degradation reactions in 2D materials

11:35am-12:00pm Ye Xu: Mapping out the decomposition pathway of furan on Pd(111)

12:00pm-12:10pm Concluding remarks; adjourn.