**SCHEDULE**

**TSRC Workshop on Stochastic Electronic Structure Methods, June 2-6, 2025**

**Note that there is a** Meet & Greet at [Alibi](https://nam12.safelinks.protection.outlook.com/?url=https%3A%2F%2Fwww.alibitelluride.com%2F&data=05%7C02%7Cjordan%40pitt.edu%7Ca504cfdcbb7c41a0446b08dd890f2f39%7C9ef9f489e0a04eeb87cc3a526112fd0d%7C1%7C0%7C638817420504983407%7CUnknown%7CTWFpbGZsb3d8eyJFbXB0eU1hcGkiOnRydWUsIlYiOiIwLjAuMDAwMCIsIlAiOiJXaW4zMiIsIkFOIjoiTWFpbCIsIldUIjoyfQ%3D%3D%7C0%7C%7C%7C&sdata=eEKoOlHJrJPIMoBePwu8m1%2FKqSM15f6K6pmcYY2UtX8%3D&reserved=0) – 157 S. Fir Street on Sunday, June 1st from 5:00 pm to 6:30 pm. If you are able to make it you can pick up your meeting badge there. Otherwise, you can pick it up at the Telluride Innovation center at 300 S Townsend St when you drop by for breakfast on Monday.

**Monday, June 2**

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| 9:00 – 9:40 AM | James Shee | *Recent developments in phaseless auxiliary-field quantum Monte Carlo for chemical systems* |
| 9:40 – 10:20 | Joonho Lee | *Auxiliary-field quantum Monte Carlo for solids in the thermodynamic limit* |
| 10:20 – 10:35 |  | *coffee break* |
| 10:35 – 11:15 | Jenny Zhan | *Neural Network Wave Functions for Spin-Dependent Hamiltonians* |
| 11:15 – 11:40 | Leon Otis | *Targeting Excited States with Auxiliary Field Quantum Monte Carlo* |
| 11:40 – 12:05 | Lucas Wagner | *Optimization of excited states in variational Monte Carlo: getting decent efficiency* |
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**Tuesday, June 3**

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| 1:00 – 1:40 PM | Ralph Wheeler | *Fixed-node diffusion Monte Carlo achieves chemical accuracy for predicting substituent effects on reaction enthalpies and activation energies for methyl radical addition to some substituted olefins* |
| 1:40 – 2:20 | Sonali Joshi | *Stable regularized loss function to learn effective model Hamiltonians from ab initio: Interacting models of the Hydrogen chain* |
| 2:20 – 2:45 | Yueqing Chang | *Downfolding from ab initio to interacting model Hamiltonians: comprehensive analysis and benchmarking of the DFT+cRPA approach* |
| 2:45 –3:00 |  | *Coffee break* |
| 3:00 –3:40 | Paul Kent | *Real space QMC at Exascale* |
| 3:40 –4:05 | Gil Goldshlager | *Accelerating stochastic reconfiguration in the few-sample, many-parameter regime* |
| 4:05-4:30 | Ryan Adams | *Accelerating MCMC on GPUs* |
| *6:30* |  | *Town Talk* |

**Wednesday, June 4**

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| 9:00 – 9:40 AM | Michael Lindsey | *A mathematical analysis of stochastic density functional theory* |
| 9:40 – 10:05 | Sandeep Sharma | *Following in the footsteps of coupled cluster to improve the accuracy of AFQMC* |
| 10:05-10:30 | Tong Jiang | *Unbiasing Auxiliary-Field Quantum Monte Carlo with Matrix Product States Trial Wavefunctions* |
| 10:30 – 10:45 |  | *coffee break* |
| 10:45 – 11:10 | Anouar Benali | *Quantum Monte Carlo in Biological Chemistry: capturing molecular response in complex environment* |
| 11:10 – 11:35 | Brenda Rubenstein | *Surrogate Forces for Quantum Monte Carlo and Quantum Computation* |
| 11:35 – 12:00 | Ken Jordan | *Configuration Interaction and DMC studies of positron-atom and positron-molecule binding* |
| 5:30-7:30 PM |  | *Picnic* |

**Thursday, June 5**

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| 1:00 – 1:40 PM | Michele Casula | *Generating accurate potential energy surfaces by quantum Monte Carlo* |
| 1:40 – 2:20 | Peter Orbanz | *Symmetrization strategies for machine learning models* |
| 2:20 – 2:45 | Lukas Weber | *Auxiliary field quantum Monte Carlo methods for cavity-coupled molecules and materials* |
| 2:45 –3:00 |  | **Coffee break** |
| 3:00 –3:25 | Eric Neuscamman | *Seeking Efficiencies in VMC Optimization* |
| 3:25 –3:50 | Amanda Dumi | *Assessing La3Ni2O7 structural properties: A quantum Monte Carlo study accelerated by the Surrogate Hessian approach* |
| 3:50-4:05 |  |  |
| 4:05- 4:20 |  |  |
| 4:20-4:35 |  |  |