**SCHEDULE**

**Telluride Science Workshop on Stochastic Electronic Structure Methods***June 5 – 9, 2022*

**Monday, June 6**

|  |  |  |
| --- | --- | --- |
| 8:55 – 9:00 AM | Mark Kozak | *General information about Telluride Science* |
| 9:00 – 9:35 AM | Claudia Filippi | *“Targeting excited states with quantum Monte Carlo”* |
| 9:35 – 9:55 AM | Ankit Mahajan | *"Excited states and properties in auxiliary field quantum Monte Carlo"* |
| 9:55 – 10:15 AM | Daniel Staros | *"Exciton binding energies in monolayer CrI3 from Diffusion Monte Carlo"* |
| 10:15 – 10:40 AM |  | **coffee break** |
| 10:40 – 11:15 AM | Eric Neuscamman | *"Can less be more in VMC optimization?".* |
| 11:15 – 11:35 AM | David Ceperley | *"The role of QMC in developing Born-Oppenheimer potentials"* |
| 11:35 – 12:00 PM |  | **discussion** |
| 1:00 - 5:00 PM |  | **Informal scientific discussion** |

**Tuesday, June 7**

|  |  |  |
| --- | --- | --- |
| 9:00 – 9:35 AM | Lucas Wagner | *TBD* |
| 9:35 – 9.55AM | Jaron Krogel | *"Addressing diffusion Monte Carlo structural relaxation and locality error"* |
| 9:55 – 10:15 AM | Amanda Dumi | *"Initial Performance of a Jastrow Factor Based on Spectral Neighbor Analysis Potentials”* |
| 10:15 – 10:40 AM |  | **coffee break** |
| 10:40 – 11:15 AM | James Shee | *“Exploring new frontiers in transition metal quantum chemistry: Synergies between AFQMC, symmetry breaking, and CCSD(T)”* |
| 11:15 – 11:35 AM | Paul Yang | *"Metal-insulator transition in transition metal dichalcogenide heterobilayer: accurate treatment of interaction"* |
| 11:35 – 12:00 PM |  | **discussion** |
| 1:00 – 5:00 PM |  | **Informal scientific discussion** |

**Wednesday, June 8**

|  |  |  |
| --- | --- | --- |
| 9:00 – 9:35 AM | Brenda Rubenstein | *"New Auxiliary Field Quantum Monte Carlo Algorithms for Probing Entanglement"* |
| 9:35 – 9:55 AM | Yannic Rath | *"Gaussian Process States - Ab initio wavefunctions from Bayesian machine learning techniques"* |
| 9:55 – 10:15 AM | Scott Jensen | *“Dense hydrogen phases from machine-learned potentials trained with Quantum Monte Carlo”* |
| 10:15 – 10:40 AM |  | **coffee break** |
| 10:40 – 11:15 AM | Cyrus Umrigar | *"Reducing the DMC time-step error of total energies and binding energies and prospects for an efficient time-step error free algorithm"* |
| 11:15 – 11:35 AM | Yueqing Chang | *"Learning emergent models from ab initio many-body calculations"* |
| 11:35 – 12:00 PM |  | **discussion** |
| 1:00 – 5:00 PM |  | **Informal scientific discussion** |

**Thursday, June 9**

|  |  |  |
| --- | --- | --- |
| 9:00 – 9:35 AM | Adrian del Maestro | *“Entanglement in Strongly Correlated Systems via Quantum Monte Carlo"* |
| 9:35 – 9:55 AM | Giacomo Tenti | *"Principal deuterium Hugoniot via Quantum Monte Carlo and Delta-learning”* |
| 9:55 – 10:15 AM | Shiv Upadhyay | *"Positron binding to neutral Beryllium clusters"* |
| 10:15 – 10:40 AM |  | **coffee break** |
| 10:40 – 11:00 AM | Anouar Benali | *“Diffusion Monte Carlo study of the de/hydrogenation energy of Liquid Organic Hydrogen Carriers”* |
| 11:00 – 11:20 AM | Kosuke Nakano | *“Recent progress in high-throughput calculations using TurboRVB”* |
| 11:20 – 11:40 AM | Ken Jordan | *TBD* |
| 11:40 – 12:00 PM |  | **discussion** |
| 1:00 – 5:00 PM |  | **Informal scientific discussion** |

**Friday, June 10**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| 9:00 – 9:35 AM | Miguel Morales | | | |  | |
| 9:35 – 9:55 AM | TBD | | | |  | |
| 9:55 – 10:15 AM | | |  | | --- | | TBD | | | | |  | | --- | |  | | |
| 10:15--10:30 AM | | |  | | | **discussion** |
| 9:45 – 10:30 AM | |  | | | **coffee break** | |
| 10:30 – 11:00 AM | | | |  | **Meeting wrap-up** | |