[**Quantum Computing for Quantum Chemistry, Molecular Dynamics, and Bey**](https://urldefense.com/v3/__https://r20.rs6.net/tn.jsp?f=001_UqS5s0QN8vBRyVZnhIvPxmJNwaJi1-R2KuQy63gjlV3ewHchRgO9mMTVc9z5Eh43FWw5Ka87DW-2UzLHcu-TOGyFNnJVmOMx5rBuws5HZySBlYOEBVZPymofIftZsLTEvOLo7CzmaIQ7_i2dr6IhqEtPAgchxmJ_Q2E1pzenKjEUr55aa6uB3X2SvIzWdyhIxXPXaigKFZMWpRgw9GXgA==&c=eUSO4Yvh3-q--Z6J_qSxso9DFUWFyheVRH1EzRYhynUjrZvWpJZkTw==&ch=xUNjr63iwJhGL1wwCC9blyxiTmJJlWg0eVX2kJX67nXcrdVKSNQP6Q==__;!!Bt8fGhp8LhKGRg!FpzA2do_A5uzN6oYovcBxGuZqmhyen-lxSwqd8JctY9X9OqIkFbbvIN3Z8VWBTDbxwJTDu1khPXNsWStmxgF1DQu$)**ond**

March 25-29, Telluride, CO

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| --- | --- | --- | --- | --- |
|  | **Monday** | **Tuesday** | **Wednesday** | **Thursday** |
| 7:55 - 8:00 AM | Opening remarks | - |  | - |
|  | **Classical algorithms** | **NISQ Algorithms** | **Fault-tolerant Algorithms** | **Algebraic and tensor train techniques** |
| 8:00 - 8:40 AM | Gustavo Scuseria | Peter Love | Di Fang | Alexander F. Kemper |
| 8:40 - 9:20 AM | Sandeep Sharma | Mario Motta | Peter Johnson | Artur Izmaylov |
| 9:20 - 10:00 AM | Avanish Mishra | Antonio Mezzacapo | Nathan Wiebe | Micheline Soley |
| 10:00-4:30 PM | Free discussion | Free discussion | Free discussion | Free discussion |
|  | **NISQ Algorithms** | **NISQ Algorithms** | **Open Systems and dynamics** | **Hamiltonian preprocessing** |
| 4:30-5:10 PM | David Munoz Ramo | Karol Kowalski | Kade Head-Marsden | Matthias Degroote |
| 5:10-5:50 PM | Daniel Chaves Claudino | Tom O’Brien | Ignacio Franco | Christian Cortes |
| 5:50-6:30 PM | Bo Peng | Nicholas Sawaya | Yu Zhang | **Group Discussion: The Future of Quantum Chemistry Simulation** |

Notes:

* TSRC is to host a Meet & Greet at [Alibi](https://urldefense.com/v3/__https://www.alibitelluride.com/__;!!Bt8fGhp8LhKGRg!DTRdxvEUxPYhwEtzYXccsVgQc5q9eCUga5dUV_F8iDZkbJqv9mDbbPM3nuW5_fgMOGQD-5gw1EdJLu85s37MMn152Q$) at 157 S. Fir Street on Sunday, March 24th from 5:00 - 6:30pm. Alibi is right next door to Baked in Telluride and across the street from the workshop venue at the Ah Haa School.
* Badges, breakfast cards, & requested ski tickets will be distributed at the Meet & Greet or at the workshop venue (155 W. Pacific Ave) before the first meeting.
* **No food of any kind will be allowed in the workshop space** due to a participant with severe airborne allergies.

**Daily schedule**

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| --- | --- | --- |
| **Sunday, March 24th – Meet & Greet at** [**Alibi**](https://urldefense.com/v3/__https://www.alibitelluride.com/__;!!Bt8fGhp8LhKGRg!DTRdxvEUxPYhwEtzYXccsVgQc5q9eCUga5dUV_F8iDZkbJqv9mDbbPM3nuW5_fgMOGQD-5gw1EdJLu85s37MMn152Q$) **(157 S. Fir Street)** | | |
| **March 25, Monday** | | |
| 7:55 - 8:00 AM | Opening remark | |
| **Classical algorithms**; chair: Artur Izmaylov | | |
| 8:00 - 8:40 AM | Gustavo Scuseria | Exploiting dualities for strong correlation |
| 8:40 - 9:20 AM | Sandeep Sharma | Using Quantum Algorithms in Classical computers |
| 9:20 - 10:00 AM | Avanish Mishra | Insight into exfoliation, functionalization, and properties of MXenes via first-principles and machine learning |
| Break | | |
| **NISQ algorithms**; chair: Yu Zhang | | |
| 4:30-5:10 PM | David Munoz Ramo | Cumulant Expansion of the Lanczos Method for the Quantum Computation of Green's Functions |
| 5:10-5:50 PM | Daniel Chaves Claudino | Post hoc corrections to unitary coupled cluster based on many-body perturbation theory |
| 5:50-6:30 PM | Bo Peng | Unleashed from constrained optimization: Quantum computing for quantum chemistry employing generator coordinate method |
| **March 26, Tuesday** | | |
| **NISQ algorithms**; chair: Bo Peng | | |
| 8:00 - 8:40 AM | Peter Love | Contextual Subspace VQE |
| 8:40 - 9:20 AM | Mario Motta | Bridging physical intuition and hardware efficiency for correlated electronic states: the local unitary cluster Jastrow ansatz for electronic structure |
| 9:20 - 10:00 AM | Antonio Mezzacapo | Recent quantum algorithms for the ground state problem |
| Break | | |
| **NISQ algorithms**; chair: Peter Love | | |
| 4:30-5:10 PM | Karol Kowalski | Quantum flow formulations and distributed quantum computing algorithms |
| 5:10-5:50 PM | Tom O’Brien | State-based quantum error mitigation for quantum simulation |
| 5:50-6:30 PM | Nicholas Sawaya | Evaluating sums of non-commuting Pauli terms using string-matching and diagonalization |
| **March 27, Wednesday** | | |
| **Fault-tolerant algorithms**; chair: Matthias Degroote | | |
| 8:00 - 8:40 AM | Di Fang | Uniform Trotter Observable Error Bounds in the Planck Constant |
| 8:40 - 9:20 AM | Peter Johnson | Early Fault-tolerant Quantum Computing |
| 9:20 - 10:00 AM | Nathan Wiebe | Quantum Algorithms |
| Break | | |
| **Open systems and dynamics**; chair: Michelin Soley | | |
| 4:30-5:10 PM | Kade Head-Marsden | Open system and parity-time symmetric dynamics on current NISQ computers |
| 5:10-5:50 PM | Ignacio Franco | Analog Quantum Simulation of the Dynamics of Open Quantum Systems with Quantum Dots and Microelectronic Circuits |
| 5:50-6:30 PM | Yu Zhang | Quantum Krylov subspace method for excited state dynamics |
| March 28, Thursday | | |
| **Algebraic and tensor train techniques**; chair: Nathan Wiebe | | |
| 8:00 - 8:40 AM | Alexander F. Kemper | Dynamical Lie Algebras for Quantum Computing |
| 8:40 - 9:20 AM | Artur Izmaylov | Algebraic techniques for quantum chemistry on a quantum computer |
| 9:20 - 10:00 AM | Micheline Soley | Tensor Trains and Quantum Computing for Highly Multidimensional Molecular Simulations |
|  |  | **Hamiltonian preprocessing**; Chair: Di Fang |
| 4:30-5:10 PM | Matthias Degroote | Classical preprocessing to speed up quantum simulation |
| 5:10-5:50 PM | Christian Cortes | Assessing the performance of quantum algorithms using symmetry-aware spectral bounds |
| 5:50-6:30 PM |  | **Group Discussion: The Future of Quantum Chemistry Simulation** |
| **The end of the meeting** | | |