**Schedule for the Stochastic Electronic Structure Methods TSRC Workshop (Please note that all times are for the Eastern Time Zone, US)** Note that the talks will be given using Zoom, while the poster sessions will be done on gather.town. The links needed to connect will be sent in a subsequent email.

# Tuesday

Excited states

10:35-10:45 AM Introductory remarks (Ken Jordan)

10:45-11:15 AM Claudia Filippi: Variational principles and excited states in quantum Monte Carlo

11:15-11:45 AM Lubos Mitas: Ground and excited states in periodic framework QMC: systematic biases and statistical errors

11:45-12:15 PM Eric Neuscamman: Variational Monte Carlo and State-Specific Quantum Chemistry

12:15-12:30 PM General discussion

Pseudopotentials and FN-DMC

1:00-1:30 PM Cyrus Umrigar: Nonlocal pseudopotentials and time-step errors in diffusion Monte Carlo

1:30-2:00 PM Andrea Zen: DLA: a new scheme for fixed node diffusion quantum Monte Carlo with pseudopotentials, improving . reproducibility and reducing the trial-wave-function bias

2:00-2:15 PM General discussion

**Wednesday**

Hydrogen calculations

10:35-10:45 AM Introductory remarks (Miguel Morales)

10:45-11:15 AM Michele Casula: Phase diagram of high-pressure hydrogen including quantum nuclear effects

11:15-11:25 AM Michele Ruggeri: Quantum Monte Carlo simulations of liquids in extreme conditions: the principal Hugoniot of deuterium

11:25-11:45 AM Vitaly Gorelov: Electronic band gaps with quantum Monte Carlo, application to hydrogen metallization

11:45-12:00 PM General discussion

Poster session A

12:30-4:00 PM

**Thursday**

Machine Learning

10:35-10:45 AM Introductory remarks (Lucas Wagner)

10:45-11:15 AM George Booth: Machine-learning inspired QMC and QMC inspired machine-learning

11:15-11:45 AM Bryan Clark: Variational Monte Carlo in the Age of Machine Learning

11:45-12:00 PM Break

12:00-12:30 PM James Spencer: Learning wavefunctions: deep neural networks for quantum chemistry

12:30-1:00 PM Matthew Foulkes: Solving the Many-Electron Schrödinger Equation with Deep Neural Networks

1:00- 1:15 PM General discussion

Poster session B

1:15-4:00 PM

**Friday**

Second quantized methods

10:35-10:45 AM Introductory remarks (Brenda Rubenstein)

10:45-11:15 AM Tim Berkelbach: Stochastic quantum chemistry with fast randomized iteration

11:15-11:45 AM Sandeep Sharma: Reducing the sign problem in AFQMC with better initial states

11:45-12:00 PM Break

12:00-12:30 PM Joonho Lee: Auxiliary-Field Quantum Monte Carlo Beyond the Electronic Ground State

12:30-1:00 PM Shiwei Zhang: Toward systematic applications of QMC in solids

1:00-1:30 PM General discussion