

# WEST COAST THEORETICAL CHEMISTRY SYMPOSIUM

Stanford University, Sapp Center, 28<sup>th</sup> March 2018

Organizers: *Martin Head-Gordon, Tom Markland, Eran Rabani and Joe Subotnik*

## 8:00 am Breakfast

## 8:45 am Welcome/Introduction

### Session 1: Chair - Lee-Ping Wang, UC Davis

- 9:00 am Raphael D. Levine, UCLA, "An Isotope Effect in the Electron-Nuclear Non-equilibrium Dynamics in N<sub>2</sub>"
- 9:40 am Daniel Levine, UC Berkeley, "Extremely Large Active-Space Calculations with Adaptive Sampling Configuration Interaction"
- 10:00 am Alexei Stuchebrukhov, UC Davis, "Concerted Tunneling of Electrons and Protons in Proteins"

## 10:40 am Coffee Break

### Session 2: Chair - David Limmer, UC Berkeley

- 11:00 am Katherine Klymko, UC Berkeley, "Towards a Thermodynamics of Continuous Active Media"
- 11:20 am Chenchen Song, Stanford, "Reduced Scaling Formulation of Multi-reference Perturbation Theory via Supporting Subspaces and Tensor Hyper-Contraction"
- 11:40 am Hans Andersen, Stanford, "Why is the Verlet Algorithm so Useful for Molecular Dynamics Simulations?"

## 12:20 pm Lunch and Poster Session

### Session 3: Chair - Evan Reed, Stanford

- 2:00 pm Anne McCoy, U Washington, "Spectral Signatures of Hydrogen-bonding: Vibrational Spectroscopy of Solvated Ions"
- 2:40 pm Christine Isborn, UC Merced, "Modeling the Absorption Spectra of Molecules in Solution: Combining the Ensemble and Franck-Condon Approaches"
- 3:20 pm Julia Rice, IBM Almaden, "Quantum Computing and Quantum Chemistry: Where are we today and what is the potential for the future?"

## 4:00 pm Coffee Break

### Session 4: Chair - Hrant Hratchian, UC Merced

- 4:20 pm Eric Neuscamman, UC Berkeley, "Interconverting Variational Principles for Excited States"
- 4:40 pm Ilan Benjamin, UC Santa Cruz, "Reactions at Liquid Interfaces: The Interplay Between Surface Fluctuations and Local Structure and Dynamics"
- 5:20 pm Thom Dunning, U Washington, "A "New" Multiconfiguration Description of Molecules"

## 6:00 pm Final Remarks/Close (Meeting ends ~6:05pm)

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