

**CHAMPS** Chemistry and Mathematics in Phase Space

US Roaming Workshop - 1st + 2nd October 2022

*"The Roaming Mechanism for Reaction Dynamics: State of the Art, Open Questions, and Future Directions"*

MSU in room CEM481,

Saturday 1st October 2022		
9.00 - 9.30	Registration + Welcome Remarks	MSU in room CEM481
9.30 - 10.10	Joel Bowman - Online Talk	"A roaming overview of "roaming"
10.10 - 10.50	Arthur Suits	"How far can a radical roam?"
Coffee Break 10.50		
11.10 - 12.00	Stavros Farantos - Online Talk	"Geometric Theories of Chemical Reactions: Classical – Quantum – Thermo - Dynamics"
Lunch 12.00		
1.00 - 1.40	Heide Ibrahim	"Directly imaging the roamer in formaldehyde using Coulomb explosion imaging"
1.40 - 2.20	Paul Houston	"QCT Simulations of Roaming Relevant to Recent Experiments on Formaldehyde"
Tea Break 2.30		
3.00 - 4.00	Marcos Dantus + Ben Levine	"Timescale of H <sub>3</sub> <sup>+</sup> formation from CH <sub>3</sub> X compounds following ultrafast ionization and astrochemical implications"
5.30 - late	Dinner - Sansu	Sansu - 4750 S.Hagadorn Rd, East Lansing, MI 48823 - <a href="https://sansu-sushi.com/">https://sansu-sushi.com/</a>

**Sunday 2nd October 2022**

9.00 - 9.30	<i>Day 2 arrival tea + coffee</i>	<i>MSU in room CEM481</i>
9.40 - 10.20	<i>Returning Remarks</i> <i>Stephen Klippenstein</i>	<i>"Multistage and Multichannel Roaming in Criegee Intermediates: Theory and Experiment".</i>
10.20 - 11.00	<i>Vladimir Krajnak – Online Talk</i>	
<i>Coffee Break</i> <i>11.00</i>		
11.30 - 12.10	<i>Markus Meuwly – Online Talk</i>	<i>Machine Learned Potentials for Reaction Dynamics.</i>
<i>Lunch</i> <i>12.30</i>		
1.30 - 3.00		
<i>Tea Break</i> <i>3.10</i>		
4.10 - 4.30	<i>Closing Remarks</i>	