

Announcing the Final Examination of William C. Tucker for the degree of Doctor of Philosophy in Physics

Date: April 5, 2019

Time: 3:00 p.m.

Room: PSB 160

Dissertation title: **Chemistry and dissipation at mineral surfaces in the space environment.**

Abstract:

The composition and morphology of mineral surfaces is known to play an important role in various phenomena relevant to planetary science. For example, the synthesis and processing of complex organics likely occurs at mineral surfaces strongly affected by the space environment. Furthermore, the dissipative and adhesive properties of dust grains may depend strongly on the chemical state of the surface including the presence of dangling bonds, adsorbates, and radicals. In this defense, results obtained using molecular-dynamics simulations demonstrate that uncoordinated surface atoms in metallic nanoparticles result in plastic deformation, strong dissipation and adhesion. This can be contrasted with previous simulations which demonstrate significantly weaker dissipation when surface atoms are passivated. Calculations of critical sticking velocities demonstrate that simple coarse-grain models are insufficient for predicting the adhesive behavior of sub-micron sized grains. To further elucidate dissipation, the direct coupling of harmonic vibrational modes in the dissipation process is established. The results demonstrate broad participation of low and high-frequency modes during a collision during a timescale less than time required for particles to rebound. Hence, our results demonstrate extremely strong likelihood of adhesion during collisions. This approach provides a way to use density-functional theory calculations to directly compute dissipative couplings at mineral interfaces. Thirdly, experimental results are presented which demonstrate that mineral grains subjected to high temperatures in a reducing environment lead to iron nanoparticles which are strongly catalytic for the complex organic species. Lastly, results are presented describing a computational study illuminating the role of surface chemistry on the adhesion and dissipation of iron nanoparticle collisions, which in the case of free radical adsorbates may also contribute to the creation of more complex species.

Outline of Studies:

Major: Physics

Educational Career:

B. S. University of Central Florida, United States, 2002

Committee in Charge:

Dr. Patrick K. Schelling (Chair)

Dr. Daniel T. Britt

Dr. Abdelkader Kara

Dr. Kevin Coffey (External Committee Member)

Approved for distribution by Dr. Patrick K. Schelling, Committee Chair, on March 21, 2019.

The public is welcome to attend.