

Tuesday, April 25, 2017

## ORIGIN AND EVOLUTION OF LIFE: PREBIOTIC CHEMISTRY:

## AB INITIO COMPUTATIONAL PREBIOTIC CHEMISTRY

10:15 a.m. Arizona Ballroom E-G

- 10:15 a.m. Goldman N. \*  
[\*Self-Assembly of Prebiotic Organic Materials from Impact Events of Amino Acid Solutions\*](#) [#3051]  
We have used quantum simulations to study the formation of oligomeric structures in impacts of aqueous glycine solutions on early Earth or other icy planets.
- 10:30 a.m. Pérez Villa A. \* Georgelin T. Lambert J-F. Rigaud B. Guyot F. Maurel M-C.  
Saitta A. M. Pietrucci F.  
[\*Ab-Initio Molecular Dynamics Simulations and NMR Experiments of RNA Nucleotides in Hydrothermal Prebiotic Conditions\*](#) [#3346]  
We model the ribonucleotide synthesis/degradation under hydrothermal prebiotic conditions by ab initio molecular dynamics combined with free-energy methods.
- 10:45 a.m. Bera P. P. \* Stein T. Head-Gordon M. Lee T. J.  
[\*Nucleobase Synthesis via UV-Induced Oxidation of Their Precursors in Astrophysical Ices: A Quantum Chemical Perspective\*](#) [#3191]  
Nucleobase synthesis via UV-induced oxidation of their precursors in astrophysical ices: A quantum chemical perspective.
- 11:00 a.m. Muralidharan K. \* Asaduzzaman A. Zega T. J.  
[\*Endogenous Source of Organics and Water in Earth-Like Planets\*](#) [#3209]  
Using theory and experiments, we demonstrate that water and organics must have been incorporated in Earth-like planets during the early stages of accretion.