Endogenous Source of Organics and Water in Earth-like Planets. Krishna Muralidharan,[1] Abu Asaduzzaman[1,2] and Thomas J. Zega[1?,3], [1]Department of Materials Science and Engineering, University of Arizona (krishna@email.arizona.edu), [2]Department of Life and Physical Sciences, Lincoln University, [3]Lunar and Planetary Laboratory, University of Arizona

Introduction: Organic compounds and water represent biocritical ingredients that are necessary for initiating and sustaining life. It has been suggested that a large amount of carbon compounds were delivered to the Earth by meteorites and comets [1] which spontaneously transformed into amino acids and other biochemical compounds. On the other hand, it has been recently shown that organic solids can directly condense from the gas phase even during the protoplanetary disk stage, suggesting that prebiotic building blocks could have been delivered during the planetary accretion stage itself [2]. In this context, there are fundamental questions regarding the timeline and nature of the delivery of such biocritical ingredients to the Earth; further by extension, could such processes be applicable to other Earth-like planets too?

Towards this end, using quantum chemical based computational methods, we examine the ability of both water molecules as well as organic compounds to be delivered during the early stages of planetary accretion. Specifically, we study and quantify the interactions of organic compounds and water molecules with mineral grains to ascertain the possibility of an endogenous source of organics and water. For our studies, we chose representative organic compounds and mineral grains (given below) that are known to have occurred in our solar nebula. We also examine the mechanisms that could lead to mineral-surface mediated synthesis of complex organic compounds such as amino acids, sugars and carbohydrates. Further, using targeted experiments, we validate the results obtained from the quantum chemical calculations in order to confirm the possibility of an endogenous source of both organics and water as well as the possible emergence of early life on Earth-like planets, from the endogenously incorporated organics.

Methods: For the computational methods, we use density functional theory (DFT) and molecular dynamics simulations (MD). Any additional details from the theory? You have some room. Experimental work was performed via temperature programmed desorption (TPD) to study the chemical binding energy of organics and water on the select mineral surfaces. The materials systems considered in this study include a host of organic molecules (hydrocarbons, amines and carboxylic group containing organic molecules) on different surfaces of olivine ($MgSiO_4$), water ice, magnestite ($MgCO_3$) and spinel ($MgAl_2O_4$).

Results and Potential Implications: The DFT studies show that water binds very strongly to all of the considered mineral surfaces. Some of these results have already been published [3] and confirm that water molecules dissociate on mineral surfaces leading to surface hydroxylation. Further, the strong binding energies also ensure that hydroxylated molecules survive high-energy collisions between small mineral grains that underlie the planetary accretion process as shown by MD simulations. TPD experiments confirm the DFT calculations of the binding energy (i.e. the adsorption energy) of water molecules on the different mineral surfaces. Further, it was also seen that while hydrocarbon molecules such as CH_4, C_2H_2, C_6H_6 are relatively weakly adsorbed, molecules containing amine and carboxylic acid functional groups bind very strongly to the modeled mineral grain surfaces, which is attributed to the electronegative nature of the N and O atoms [4]. Such trends are also seen for alcohol, aldehyde, and amide containing organics, further confirming the important role of functional groups on the binding strength of organics on mineral surfaces. Finally, based on DFT results, it is also seen that amino acids such as gycine as well as sugars such as glycol can be readily synthesized from their constituent building blocks (e.g. amines, alcohols) catalyzed by the mineral surfaces. Specifically, it is seen that the activation barriers for the formation of complex amino acids and sugars on mineral surfaces is significantly lowered as compared to the barriers associated with the corresponding gas-phase reactions. In other words, inorganic mineral-grain surface can catalzye and mediate the self assembly of more complex biocritical compounds such as amino acids and sugars. These results, while preliminary have important implications for current theories regarding the emergence of life on Earth and Earth-like planets.

References: [1] Oró J. (1961) *Nature*, 190**,** 389-390. [2] Kwok S. and Zhang Y. (2011) *Nature*, 479**,** 80-83. [3] Asaduzzaman et al. (2013) *Phil. Trans Royal Soc. A* 371 20110582, [4] Asaduzzaman et al. (2014) *EPSL*, 408, 355.