1. **Project Title (maximum 150 characters): \***

Life in the universe: a quantum chemistry point of view

1. **Executive Summary (maximum 1300 characters): \*** The Executive Summary should briefly address the following questions:
* (a) What specific questions will your project answer?
* (b) What activities will you carry out to answer those questions?
* (c) Why is this project needed?
* (d) What concrete deliverables will you produce by the end of the project?
* (e) What impact will your project have?

How did life on earth formed ? are we alone in the universe ? These question are centeral in sceine. **If chemical evolution occurs in the interstellar medium (ISM) to form life’s building blocks, then it is possible that life is a universal phenomenon.** Understanding of the chemistry taking place in the ISM, and how prebiotic moleculse are formed is essential to our understanding of life. We propose to develop new theoretical capabilities that will enable the model of molecules in their excited electronic state due to interaction with UV radiation, a processes that is crucial to understanding interstellar chemistry. Quantum chemistry is essential for the study of interstellar chemistry, however, it is lacking the ability to model large molecules in an electronically excited state. By the end of the project, we will develope new capabilities within the framework of ensemble density functional theory that will provide the ability to model reaction of large moleculae in an excited state. We will use small systems to benchmark the new method and to prove it accuracy. The impact is expect to be tremenudus as we will, for the first time ,be able to *fully* study the possibility for formation of life’s building blocks in different outer space environment.

1. **Project Description (maximum 4000 characters including everything): \*** Please describe the work/activities you will undertake in your project.

Formation of molecules in areas like molecular clouds, the birth place of stars still puzzles scientis. Mechanism for formation of new molceuls can be considered via ‘bottom-up’ chemistry or ‘top-down’ chemistry. In the bottom-up mechanism, molecules are gradually build from smaller building block. The mechanism is used to model reactions taking place in different areas of the ISM and provide relvent astrochemical and astrobioligical insights. Moreover, quantum chemistry is used to illuminate reactions mechanism and provide molecular level undersading of chemical processes.(Bera et al. 2017) On the other hand, in the interstellar medium (ISM) molcuels speculate to also synthesized via top-down mechanism.(Candian, Zhen, & Tielens 2018). Acording to this mechanism, large aromatic moleculs can form in the stellar ejecta of asymptotic branch star. PAHs are highly excited electronically due to interaction with UV radiation. Becase they are highly excited, they freagment into smaller molecues via the top down mechanism. Excited electronic states are likely to play a crucial role in the chemistry of the ISM not only by the top down mechanism but also from the bottom-up approach. It has been shown that excited oxygen atom can further react via insertion reactions to form more comlex organic molecules and the photochemistry that occurs due to exposure of ices to UV radiation could results in formatiomn of comlex organic molecues such as amono acid. (Bergner at al, 2017) From a theoretical point of view, to model an excited electronic state potential is much more challenging then to model the ground state potential. The goal of this proposal is to develop new method, that will be both accurate and computationaly feasible to study large molecules.

The limitation in the study of fragmentation of small molecular systems is due to the fact, that density functional theorey (DFT) which is in many cases the method of choice, can not realiably model fragmentation from an excited state due to the lack of multireference caharachtere in the approximate exchange correlation (XC) functionals. We will use the formalism of ensemble DFT to study excited states. Ensemble DFT has proven useful to study excited states, however challenges arise due to the fact that the traditional XC functionals are not suffieceient in the ensemble treatment. To overcone this limitation , we will use XC functionals from generalized Kohn Sham (GKS) formalism. We will focus on the following questions:

* What features of the exact XC functional are important in ensemble treatment in order to obtain multi-reference character ?
In order to overcome the lack of multirefernce character in traditional DFT we are using ensemble DFT. As ensemele DFT uses the energy at fractional occupation numbers, the energies at fractional occupation should be correct. The energy of the exact XC functional as a function of occupation number is linear, a feature that is not obeyed using traditional functionals. However, this can be reconstruct using GKS formalism using range-separated hybrid functionals.(Kronik et al. 2012) We will study several range-separeted functionals and benchmark them with respect to high level *ab-initio* methods such as CASSCF and CASPT2 on small molecular systems, to verify that we are restoring the multirefernce character. The effect of other excat conditions such as behavior at fractional spins will also be tested on model systems.
* We will incorporate the ensemble DFT together with *ab-initio* molecular dynamic (AIMD) simulations to gain the abitlty to study the evolement of molecular systems with time. This will provide us with predictive power: under certain conditions and starting points, what molecules are form or break ?

Aquiped with the tools above we will study the formation of prebiotic molecuels on different ices composiotions doped with small aromatic moleculs. We will be able to predict astrobiological important routes for molecular formatiom.

**4. Statement of significance (maximum 1,300 characters including everything)**

Describe the current conditions in the field(s) relevant to the project, identify the problems that the project will address, and articulate the specific opportunity that your project presents.

A large multidisciplinary efforts is taking place in order to study the formation of life’s building blocks; from astronomical measurments and experiments done in labs to mimic the conditions in outer space to quantum chemistry models which study the underlying molecular mechanism. NASA lounch new telescope, the most powerful one to date, James Webb Space Telescope (JWST) on 11/21 which expected to provide a leap in our current knowelde. Theoretical calculations are crucial, as they provide insights into the uniqe chemistry that occur in outer space and can guide astronomers in their search of new molecules and provided detailed mechanism of how they got there.

To fully and accurately model the chemistry in the interstellar medium, one needs to be able to model photochemical reactions. We will developed method that will enable the study of excited state reactivity and will significantly advance the ability to model chemistry in the outer space. This is expected to have a large impact in the astrochemistry, astronomy and astrobiology communities, as well as in the chemistry community in general, as the interaction of light with matter is in the heart of many chamical processes.

**5. Outputs (1300 characters)** Outputs (sometimes called "deliverables") are important events and work products that your Project activities (described in #3, above) will lead to, and which are necessary in order for you to make progress towards your proposed Outcomes (#6 below). Please provide a list of the outputs you intend to produce.

By the end of the project, we will be capable to model reactions on excited electronic state, and to model molecular fragmentation from different excited electronic states, proceses that are in the heart of interstellar chemistry and are crucial to understand formation of prebiotic molecules in ice environments.

* We will compare the preformenace of range-separated hybrid functionals used in an ensemble formalism to the performance of traditional functionals, and compare to accurate *ab-initio* methods to examine what properties of the exact XC are crucial for modeling multirefernce characher.
* The new approach will be programed into the Qchem software, which Dr. Stein is one of the developers, to be used in *ab-initio* molecular dynamic. This will enable broad use of the new developed method so other groups can use it.
* We will preform AIMD simulations that will model conditions of different interstellar environments, and provide insght into the feasible astrobiological paths.

**6. Outcomes (1300 characters)** Outcomes (sometimes called goals, results, or impacts) are the specific and identifiable changes that you expect your Outputs will bring about (or contribute to bringing about) within 5 years of your project's end date. These should describe what the success of your project would look like. Please provide a list of the outcomes you expect to come about as a result of your outputs.

* Within 5 years of the project’s end date, the ability to model excited state reactivity accurately for large molecular systems will be computationaly feasible, and available via commercial quantum chemistry software to enlarge the use of it.
* We will be able to predicy what prebiotic molecules can form in the known conditions of moleculare clouds.
* We will have the ability to compare the feasibility of different suggersted mechanism such as the ‘top-down’ and ‘bottom-up’.
* We will work in close collaborations with experimental groups and guide their search for prebiotic molecules, as we will be able to predict the likely hood of formation of different molecules in different areas.
* The ability to model accurately excited states systems will enlarge the scope of quantum chemistry not only is astrobiological applications, as the interaction of light with material is in the heart of chemistry and material sciences.

**7. Capacity of success (1300 characters)** The Capacity for Success should explain why your team and/or organization is positioned to be successful in this project.

Dr. Tamar Stein is a specialist in quantum chemistry, and through her career developed new methoods in order to overcome the limitanions of the available tools quantum chemistry, and succesfuly broden the filed’s domain. Her work made a large impact, as expresses by the large number of citations she gained (5060). During her time as a postdoctoral fellow, Stein was part of NASA ames astrobiolgy center, and thus she is also an expert in the field of astrochemistry and astrobilogy. Dr. Stein, with her in depth knowledge of both of the fields is intimately aware of the challenges in modeling astrochemical systems, and has the capabilities to develop new method to overcome those limitations.

**8. Relation to Sir John Templeton's Donor Intent (maximum 1000 characters): \***

 Sir John Templeton motto for his foundation “How little we know, how eager to learn”, the question of formation of life is the universe is an excelent example to this motto. Very little is know about how life is formed and wehter it is form in different places of our universe. However, we are very eager to learn! These questions intrigued mankind and ignited the imagination, not only of scientist, but also authors (as is evident by the large number of science fiction books) and artist. We are hopong that the suggested project will significantly advance out understanding in the field.

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**5. Project Relationship to Previous Grants (2000 characters): \*** To the best of your knowledge, is the work of your proposed project similar to, a continuation of, or an expansion of an active or completed grant you or your organization received from either the John Templeton Foundation, the Templeton Religion Trust, or the Templeton World Charity Foundation? If "Yes," please explain your answer in the text box. Be sure to include the previous project's Title, Grant ID#, Grant Amount, end date, and a very brief synopsis of the project activities

 Dr. Tamar stein is a young pre-tenured PI, who wants to use her expertise to answer the important and big questions of humanity. This is her first grant application with the Tempelton foundation.

**13. History with the Foundation (maximum 1000 characters): \*** Please describe how you or any members of your team came to learn about the Foundation, including past grants, participation in Foundation-sponsored events, and/or discussions with staff about the project idea.

Althoug this is our first application to the foundation, as I do not have any history with it, I deeply identify with the foundation cause and will be very happy to take part foundation event.

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Bera, P. P., Stein, T., Head-Gordon, M., & Lee, T. J. 2017, Astrobiology, 17, 771

Candian, A., Zhen, J. F., & Tielens, A. G. G. M. 2018, Phys Today, 71, 38

Kronik, L., Stein, T., Refaely-Abramson, S., & Baer, R. 2012, Journal of Chemical Theory and Computation, 8, 1515