NASA is interested in the development of highly advanced systems, subsystems, and components for use with high-power, fission power and propulsion systems for a variety of future robotic and manned exploration missions, including in-space, lunar-surface, and Mars-surface applications. Advanced high-power space nuclear power and propulsion systems for robotic and human exploration missions involve a range of specialized materials for the reactor, heat transfer system, energy conversion system, propulsion system, and other nuclear vehicle systems. These materials may include carbon-carbon, super alloys, refractory alloys, structural ceramics, ceramic matrix composites, and other high-temperature space nuclear systems materials. Long-term stability greater than 10 years is critical for long-life space nuclear power system applications. Materials would be subjected to fission process radiation while exposed to in-space (plasma, out-gassing, etc.) and/or planetary operating environments.

This subtopic is focused on the development of computational materials science tools to develop and select these specialized space nuclear systems materials. Many considerations go into selection of materials for demanding applications. These include strength, creep resistance, phase stability, oxidation/corrosion resistance, nuclear capture cross-section, and radiation tolerance. In recent years computational materials science has assisted with not only the selection of existing materials with a given set of properties but also with the development of new materials with those properties. These tools include first principles calculations of phase equilibria, computational thermodynamics (the CALPHAD technique), and creep modeling.

Proposals are sought for the specific technologies areas:

- A computational 'toolbox' for material selection with particular emphasis on space nuclear power and propulsion systems requirements;
- Computational tools to address particular issues in mechanical property degradation in space nuclear power and propulsion systems over long times. This includes, but is not limited to, long-term creep modeling;
- Computational tools to predict long-term oxidation/corrosion and flow-induced erosion issues in the high temperature portions of these systems, including the heat transfer system. This includes thermodynamic
modeling of heat transfer media attack of alloys;

- Computational tools to predict long term stability of various joining techniques used in these space nuclear systems. This includes diffusion modeling in alloys; and

- Computational tools to predict interaction of the radiation environment. This includes effective capture cross-section for complex materials systems and production of secondary energy and potential impact on components.

It is anticipated that Phase 1 will focus primarily on the new computational tools for material selection and development with some limited experimental verification. Later phases should involve more extensive verification, to the point where these tools could be readily utilized for the design of space nuclear systems.