range 0.4-1 μm. This will be accomplished using the classifier described in section 3.1.1. Each representative spectrum will be associated with the cluster that it most closely resembles. The materials within this cluster will be used to provide initial estimates of potential components for the modeling effort.

### 3.2 THEORETICAL MODELING OF OBSERVATIONAL DATA

Hapke [1981, 1993 and references therein] developed a series of equations that provide the ability to calculate the reflectance of particulate surfaces. Let i be the angle of the incident light ($\mu_o$=cos i), e the angle of emergent light ($\mu$=cos e), g the phase angle between i and e, $\bar{w}$ the average single scattering albedo of the surface, B(g) the opposition surge (related to the microstructure of the surface, e.g. porosity, particle size distribution, and compaction rate with depth), P(g) the average particle phase function, and H($\mu$) and H($\mu_o$) are Chandrasekhar's H-functions [Chandrasekhar, 1960], then the bidirectional reflectance of a surface is expressed as

$$r(i,e,g,\bar{w}) = \frac{\bar{w}}{4\pi}\frac{\mu}{\mu_o+\mu}\{[1+B(g)]P(g)+H(\mu)H(\mu_o)-1\}, \quad (1)$$

$\bar{w}$ is related to the optical constants, *n* and *k*, of each component in a mixture [Hapke 1981, Clark and Roush 1984, Roush 1994, Roush et al. 1996] and hence is indicative of composition. The various assumptions contained within the Hapke-formalism (Hapke 1993, and references therein), used here are discussed in equations 1-6 of Roush (1994) and equations 1-4 of Cruikshank et al. (1997).

The approach is to model observations of solar system objects using equation 1 [e.g. Roush et al 1990, Calvin and Clark, 1991, 1993, Cruikshank et al. 1993, 1997, 1998a,b,c, Owen et al. 1993, 2001, Calvin et al. 1994, Wilson et al. 1994, Roush 1994, Wilson and Sagan 1995, Roush et al. 1996]. In our modeling efforts, the grain sizes and relative abundances of the candidate materials are adjusted, both iteratively and automatically (using a Simplex algorithm based upon Press et al. [1992], so as to minimize the differences between the resulting calculated albedos and the observations in a $\chi^2$ sense. In this process, a range of parameter space is explored by different initial conditions for the Simplex and the results near the minimal $\chi^2$ value can provide estimated uncertainties associated with the derived grain sizes and diameters.

This approach has been successfully applied during previous funding cycles to derive compositional information for various icy satellites, TNOs, and Centaur objects [Bauer et al. 2002a,b; Poulet et al. 2002; Cruikshank et al. 2003; Buratti et al. 2005; Cruikshank et al 2005; Cook et al. 2007; Olkin et al. 2007; Brunetto et al. 2007; Brunetto and Roush 2008; Pinilla-Alonso et al. 2009]. We leverage the previous investment that has resulted in the mature nature of the computer programs based on the Hapke modeling approach and will use it here for modeling of selected spectra. The proposed effort is different from the previous compositional modeling in that it uses the results of the statistical classification of the observational data to select initial candidates for the compositional modeling.

Brunetto et al. [2007] investigated models to explain the visible and near-infrared spectral behavior of irradiated silicates and found that the observed reddening and darkening spectral trend is compatible with the Hapke's space weathering model [Brunetto et al. 2007, and references therein], using the optical constants of metallic iron in a silicate matrix. The computer codes necessary for this modeling is available for our use. When the classification indicates metals as a potential component we will include such models in our efforts.

For the Trojans we will also undertake modeling the layered situations described in section 2.3. Brunetto and Roush [2008] implemented a layered reflectance model based upon Hapke's approach [Hapke 1993] and investigated the impact of a hydrocarbon residue overlying a substrate of water ice and found layers with thicknesses of 5-50 μm, depending upon the layer composition, can readily mask the distinctive spectral signature of the underlying water ice. These computer codes are available for the proposed effort. The model parameters are the reflectance of the substrate material, the reflectance of an infinite thickness of the layer material, the thickness of the substrate, and a parameter associated with how continuous (patchy) the layer is. The first two values are readily calculated using our standard computer programs. The minimum thickness of the layer will be constrained to be equivalent to the diameter of the grains composing it and the maximum will be determined when there is no residual signature present from the substrate. We will use a continuous layer for all our calculations.

## 4. PLANNED WORK

### 4.1 Statistical Clustering of Observational & Laboratory Data

*4.1.1 Statistical Clustering of Laboratory spectra containing organics*

**Collection of Available data and Preparation of Data for Statistical Analyses** (Task 1) – The spectra of a variety of organic-bearing materials are available within the RELAB spectral data base [http://lf314-rlds.geo.brown.edu]. However, significant discrepancies exist in how these spectra are labeled as organics. For example, some are clearly labeled as organics, other as man-made, and in several cases mention of organics is only provided in the sample description. The RELAB provides two Microsoft Excel spreadsheets. One contains the sample description and the other the links to the spectral information. While some aspects of sorting out these sample label discrepancies can be automated, e.g. searching for "organic", cross correlating it with entries in the other Excel document can not. Each sample potentially contains multiple measurements at different wavelengths. This simple gathering together of appropriate data is labor intensive. As a result, it will require some additional time in the first year to evaluate the inclusion of organics into a spectral library for clustering. Without a priori knowledge of the number of potential samples, it is difficult to provide an accurate time estimate required for this effort. We estimate 4-6 weeks for this effort in the first year.

Cruikshank et al. [1991] present the spectra of a variety of hydrocarbons. Moroz et al. [1996] present spectra of naturally occurring terrestrial organic materials. We have both of these data sets and they will be added to the spectral library used for clustering. Moroz et al. [1998] obtained spectra for 15 solid bitumens over the 0.5-16 μm wavelength range. We will contact Moroz to get digital versions of these data to include in our analyses. This effort is not estimated to require a significant effort.

After the collection of the appropriate spectra of organic materials, we will follow the approach of Roush and Hogan [2007] and Marzo et al. [2009]. We will include the new data in the composite library previously used to train our classification scheme for identification of silicates, salts, and oxides. This effort involves an appropriate re-sampling of the all spectral data to common set of wavelengths. We estimate this effort will require on the order of 1-2 weeks.

**Statistical Clustering** (Task 2) - Once the spectral library is complete statistical cluster analyses will begin. We will undertake three specific analyses.

1. Perform the analysis using data in the 0.4-1 μm wavelength region
2. Perform the analysis using data in the 0.4-2.5 μm wavelength region
3. Perform the analysis using data in the 0.4-15 μm wavelength region