Planets are born in protoplanetary disks, which means that their structure and composition are determined by and highly connected to the chemical composition and structure of the disk in which they form. In my and previous research, I have approached this intricate disk-planet link from two directions: (1) by exploring the core accretion mechanism, specifically calculating the minimum required core mass to form a gas giant before the dissipation of the gas in the protoplanetary disk, and (2) by understanding how disk chemistry and dynamics shape the snowline locations of volatiles in disks, which has direct implications for the chemical composition of extrasolar planet (exoplanet) atmospheres.

1. Minimum Core Masses for Giant Planet Formation

Gas giants are widely believed to form through core accretion, a theory in which solid protoplanetary cores grow large enough to accumulate a massive atmosphere. Core accretion is particularly challenging in the outer parts of a disk, where long dynamical times make it difficult for a core to grow fast enough before the gas disk dissipates on a timescale of a few million years. At the same time, however, giant planets on wide orbits have been discovered in recent years, which poses the question of how these planets have formed. I addressed this issue by calculating the minimum (critical) core mass M\_crit required to form a giant planet during the lifetime of the protoplanetary disk – this minimum applies when envelopes accrete around fully formed cores. To obtain robust quantitative results for M\_crit, I assumed a realistic equation of state (EOS) for the nebular gas and realistic opacities that take into account grain growth. I found that M\_crit decreases with semimajor axis, from 8 Earth masses at 5 AU to 5 Earth masses at 100 AU. These results are lower than the typically quoted value of 10 Earth masses and may be up to one order of magnitude lower if grain coagulation is taken into account. Thus my study clearly challenges previous claims that core accretion cannot operate in the outer parts of protoplanetary disks, reopening the case for in situ formation of wide-separation gas giants.

This project was conducted at Harvard University between 2012 and 2014, in collaboration with Dr. Ruth Murray-Clay and Dr. Andrew Youdin.

2. Snowlines in Protoplanetary Disks and C/N/O Ratios

The locations of volatile snowlines in protoplanetary disks are a defining feature of both gas giant and disk chemistry, as they provide vital information about the abundance of these molecules in gas and dust throughout the disk. In this part of my dissertation, I wanted to understand the effect of disk dynamical and chemical processes on volatile snowline locations and molecular abundances.

I first focused on the main carbon (C) and oxygen (O) bearing molecules, i.e H2O, CO2 and CO. The C/O ratio is an important signature of exoplanet atmosphere and disk chemistry, as small variations of the C/O ratio may affect the abundance of other volatiles by several orders of magnitudes. An important consequence of volatile condensation and sublimation in disks is that disks are expected to present different C/O ratios in the gas and in the icy dust mantles at different disk radii. I explored the effect of disk dynamics, specifically radial drift of solids and viscous gas accretion onto the central star, on snowline locations. I obtained a powerful result: these two processes alone may move the H2O, CO2 and CO snowlines inward by a factor of ~2 compared to a static disk in which these effects are not considered. This affects the C/O ratio in gas and dust throughout the disk, and thus has direct implications in shaping the composition of nascent giant planets. At the same time, these effects introduce an uncertainty of a factor of ~2 in the snowline locations of the main C and O carriers.

In addition to disk dynamics, icy particles can have different compositions: they can be pure ices, or they can reside in a water dominated environment. Since water is the least volatile species that is abundant in disks, water-dominated ices will have higher binding energies than if they are pure ices. This is particularly important for CO, as due to its high volatility, its binding energy is very different from that of water. This difference in binding energies will change the CO desorption temperature, and therefore snowline location, depending on its binding environment. Laboratory studies have shown that the CO binding energy is up to a factor of ~2 higher when CO is in a water dominated environment rather than pure ice. By applying these results to my model, I found that the ice composition may change the CO snowline location by a factor of 3-4. It thus follows that the dynamical effects described in the paragraph above together with ice compositions can change the location of the CO snowline by a factor of 7! For my particular disk model, the CO snowline can span anywhere between 9 and 61 AU. This is a very large uncertainty in the CO snowline location, and therefore in the regions of the disk where the C/O ratio is enhanced compared to the stellar value (the gas-phase C/O ratio is enhanced by a factor of 2 compared to the stellar C/O between the CO2 and CO snowlines). I thus looked into additional species or elemental ratios that could potentially better constrain this uncertainty.

Aside from the main C and O carriers, nitrogen (N) bearing species are important to study. Nitrogen is highly abundant in the Solar system and disks, and primarily found as N2. Because of the high volatility of N2, gas phase nitrogen-to-oxygen (N/O) ratio in the outer disk may be even more enhanced than the C/O ratio. Giant planets that form at wide separations should thus have an excess of N in their atmospheres, which could be used to trace their formation origin. By quantifying this effect in disks, I found that the gas-phase N/O ratio is enhanced by a factor of 2 outside the H2O snowline, by a factor of ~3 between the CO2 and CO snowlines, and by many, many orders of magnitude between the CO and N2 snowlines, where oxygen gas is practically depleted. Thus N/O ratios could be used in addition to C/O ratios to better constrain disk and giant planet compositions. As N2 has a similar binding behavior to CO, disk dynamics and ice composition may also change the location of the N2 snowline by a factor of 7.

This project has led me to two main conclusions. The first one is that gas phase N/O ratios are highly enhanced throughout most of the disk compared to the average value, and more enhanced than the C/O ratio, which means that, in principle, both C/O and N/O ratios could be used to constrain disk and planet chemical compositions. On the other hand, my second conclusion is that the locations of the CO and N2 snowlines are highly uncertain and can span several tens of AU due to disk dynamics and ice compositions. It follows that observations are KEY if we want to better understand and constrain disk and planet chemical compositions. From the theoretical standpoint, exploring other disk dynamical processes, as well as coupling disk dynamics and chemistry, has a high potential of shedding some light onto these uncertainties, which is part of what I propose to do as an NASA Postdoctoral Fellow.

This project was conducted at Harvard University between 2014 and 2016, in collaboration with Prof. Karin Oberg, Prof. Ruth Murray-Clay, Dr. Til Birnstiel and Ms. Jamila Pegues.