SOFIA PROPOSAL 08_0038

HyGAL: characterizing the Galactic interstellar medium with hydrides

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Scientific Category: ISM AND CIRCUMSTELLAR MATTER
Scientific Keywords: ABSORPTION LINES,INTERSTELLAR AND INTERGALACTIC MEDIUM,MOLECULAR CLOUDS

Abstract

By means of absorption-line spectroscopy towards 22 background terahertz continuum sources widely distributed within the Galactic plane, we will obtain robust measurements of the column densities of six hydride molecules (OH+, H2O+, ArH+, SH, OH and CH) and two key atomic constituents (C+ and O) within the diffuse ISM. Recent studies with Herschel have demonstrated the unique value of specific hydride molecules as quantitative diagnostic probes of the H2 fraction, the cosmic-ray ionization rate, or of “warm chemistry” associated with the dissipation of interstellar turbulence in regions of elevated temperature or ion-neutral drift. These observations will allow us to address several related questions: (1) What is the distribution function of H2 fraction in the ISM? (2) How does the density of low-energy cosmic-rays vary within the Galaxy? (3) What is the nature of interstellar turbulence (e.g. typical shear or shock velocities), and what mechanisms lead to its dissipation? Because of atmospheric absorption, the transitions to be observed in this program are inaccessible from the ground and can only be observed from airborne or satellite observatories. Our investigation is synergistic with ancillary observations of non-hydride molecules that have been/will be performed with ALMA, JVLA, the IRAM 30 m telescope, and APEX. There is a very timely synergy with theoretical models for H2 formation within the turbulent ISM, several of which are under development by groups within our team. The anticipated results are (1) a determination of the distribution function for the H2 fraction in the Galaxy, and how it varies; (2) a determination of the cosmic-ray ionization rate and how it varies; (3) an improved characterization of turbulence in the diffuse ISM, and its dissipation; (4) the provision of enhanced data products that will serve as a legacy for future ISM studies

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Legacy Program requested.

Related Proposals

Status of SOFIA Observations in the Last Two Years

The PI is the Principal Investigator of approved programs 06-0015, 06-0017, and 06-0022. Data acquisition is complete for all three programs. Program 06-0015 ("Terahertz water masers") yielded detections of the 1.296 THz water line, a predicted maser transition, toward 2 evolved stars: the data are currently being analysed, together with ancillary data obtained simultaneously at APEX and Effelsberg. Program 06-0017 ("Probing the molecular hydrogen fraction in diffuse molecular clouds with observations of HCl+") yielded HCl+ detections along three sightlines to bright continuum sources: the data are currently being analysed. Program 06-0022 ("Kinematics of shock-heated H2 with EXES") yielded the first detection of an H2 ortho-to-para shift toward a molecular shock, providing among the most compelling evidence to date for C-type shocks in which the flow parameters vary continuously. The results have been published in the Astrophysical Journal Letters.

Special Instructions

Instruments Requested:

Instrument	Observing Time (hr)
GREAT	71.87

Total observing time requested = 71.87 hours

Summary of AORs

Object	RA	Dec	Inst.	Config	Mode	SpectralElements	Waveln/Freq	ObsTime	Overhead	Total Time	Notes
							(μm/GHz)	(seconds)			
G09.622+0.19	18 06 14.90	-20 31 37.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
G09.622+0.19	18 06 14.90	-20 31 37.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
G09.622+0.19	18 06 14.90	-20 31 37.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
G10.47+0.03	18 08 38.40	-19 51 52.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
G10.47+0.03	18 08 38.40	-19 51 52.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
G10.47+0.03	18 08 38.40	-19 51 52.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
G19.61-0.23	18 27 38.00	-11 56 39.5	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
G19.61-0.23	18 27 38.00	-11 56 39.5	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
G19.61-0.23	18 27 38.00	-11 56 39.5	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
G291.579-00.431	11 15 05.76	-61 09 40.8	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
G291.579-00.431	11 15 05.76	-61 09 40.8	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
G291.579-00.431	11 15 05.76	-61 09 40.8	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
G31.41+0.3	18 47 34.10	-1 12 49.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
G31.41+0.3	18 47 34.10	-1 12 49.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
G31.41+0.3	18 47 34.10	-1 12 49.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
G32.80+0.19	18 50 30.63	-0 02 00.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
G32.80+0.19	18 50 30.63	-0 02 00.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
G32.80+0.19	18 50 30.63	-0 02 00.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
G328.307+0.423	15 54 07.20	-53 11 40.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
G328.307+0.423	15 54 07.20	-53 11 40.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
G328.307+0.423	15 54 07.20	-53 11 40.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
G357.558-00.321	17 40 57.19	-31 10 59.3	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
G357.558-00.321	17 40 57.19	-31 10 59.3	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
G357.558-00.321	17 40 57.19	-31 10 59.3	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
G45.07+0.13	19 13 22.00	10 50 54.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
G45.07+0.13	19 13 22.00	10 50 54.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
G45.07+0.13	19 13 22.00	10 50 54.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
HGAL0.55-0.85	17 50 14.52	-28 54 30.7	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
HGAL0.55-0.85	17 50 14.52	-28 54 30.7	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
HGAL0.55-0.85	17 50 14.52	-28 54 30.7	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	

Summary of AORs

Object	RA	Dec	Inst.	Config	Mode	SpectralElements	Waveln/Freq	ObsTime	Over head	Total Time	Notes
							(μm/GHz)	(seconds)			
HGAL284.015-0.	18 56 03.68	-0 51 27.6	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
HGAL284.015-0.	18 56 03.68	-0 51 27.6	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
HGAL284.015-0.	18 56 03.68	-0 51 27.6	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
HGAL285.26-0.05	10 31 29.48	-58 02 19.5	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
HGAL285.26-0.05	10 31 29.48	-58 02 19.5	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
HGAL285.26-0.05	10 31 29.48	-58 02 19.5	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
IRAS 12326-6245	12 35 35.90	-63 02 29.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
IRAS 12326-6245	12 35 35.90	-63 02 29.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
IRAS 12326-6245	12 35 35.90	-63 02 29.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
IRAS 15520-5234	15 55 48.70	-52 43 05.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
IRAS 15520-5234	15 55 48.70	-52 43 05.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
IRAS 15520-5234	15 55 48.70	-52 43 05.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
IRAS 16060-5146	16 09 52.41	-51 54 58.5	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
IRAS 16060-5146	16 09 52.41	-51 54 58.5	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
IRAS 16060-5146	16 09 52.41	-51 54 58.5	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
IRAS 16164-5046	16 20 11.90	-50 53 17.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
IRAS 16164-5046	16 20 11.90	-50 53 17.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
IRAS 16164-5046	16 20 11.90	-50 53 17.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
IRAS 16172-5028	16 21 03.70	-50 35 23.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
IRAS 16172-5028	16 21 03.70	-50 35 23.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
IRAS 16172-5028	16 21 03.70	-50 35 23.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
IRAS 16183-4958	16 22 10.10	-50 06 06.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
IRAS 16183-4958	16 22 10.10	-50 06 06.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
IRAS 16183-4958	16 22 10.10	-50 06 06.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
IRAS 16352-4721	16 38 50.60	-47 28 04.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
IRAS 16352-4721	16 38 50.60	-47 28 04.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
IRAS 16352-4721	16 38 50.60	-47 28 04.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
IRAS 16547-4247	16 58 17.21	-42 52 08.9	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	

Summary of AORs

Object	RA	Dec	Inst.	Config	Mode	SpectralElements	Waveln/Freq	ObsTime	Overhead	Total Time	Notes
							(μm/GHz)		(seconds)		
IRAS 16547-4247	16 58 17.21	-42 52 08.9	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
IRAS 16547-4247	16 58 17.21	-42 52 08.9	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
W3 IRS 5	2 25 40.54	62 05 51.4	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
W3 IRS 5	2 25 40.54	62 05 51.4	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
W3 IRS 5	2 25 40.54	62 05 51.4	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	
W43 MM1	18 47 47.00	-1 54 28.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_4G	4744.77749	3600	3720	7320	
W43 MM1	18 47 47.00	-1 54 28.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	1200	1320	2520	
W43 MM1	18 47 47.00	-1 54 28.0	GREAT	DUAL-CHAN	BSW	GRE_HFA GRE_LFA	4744.77749	900	1020	1920	

--- End of Proposal Summary ---

SCIENTIFIC CONTEXT

Context: In theories for star formation, a crucial missing link remains the process by which molecular clouds (the sites of star formation, traced by CO) form out of the atomic medium, and the timescale on which molecular cloud formation occurs.

The proposed investigation will address several related questions about the interstellar medium (ISM) and star formation:

- What is the distribution function of H_2 fraction in the ISM in different environments; and what are the mass fractions of (a) diffuse *atomic* gas, (b) "CO-dark" diffuse *molecular* gas, and (c) *dense* molecular gas?
- How does the density of low-energy cosmic-rays – which heat and ionize the ISM, and may play a role in regulating star-formation – vary within the Galaxy; and to what extent does the cosmic-ray density vary statistically on small scales and systematically with Galactocentric distance and gas column density?
- What is the nature of interstellar turbulence (e.g. the typical shear or shock velocities), and what mechanisms lead to its dissipation?

Aims: Our aim is to address these key questions through observations of light hydrides, i.e. molecules that contain one or more hydrogen atoms and just one heavy element atom. Such molecules lie at the root of interstellar chemistry, and are the first to form as diffuse atomic material begins its transition to the molecular phase. Recent studies with *Herschel* have demonstrated the unique value of specific hydride molecules as quantitative diagnostic probes of the H_2 fraction, the cosmic-ray ionization rate, or of "warm chemistry" associated with the dissipation of interstellar turbulence in regions of elevated temperature or ion-neutral drift.

Methods: By means of absorption-line spectroscopy towards 22 background terahertz continuum sources widely distributed within the Galactic plane, we will obtain robust measurements of the column densities of six hydride molecules (OH^+, H_2O^+, ArH^+, SH, OH and CH) and two key atomic constituents (C^+ and O) within the diffuse ISM. Because of their small reduced mass, light hydrides possess large rotational constants; their rotational transitions therefore lie at higher frequencies than non-hydrides, in spectral regions where Earth's atmosphere is opaque. Indeed, the transitions to be observed in this program are inaccessible from the ground and can only be observed from airborne or satellite observatories.

Synergies: Our investigation is synergistic with ancillary observations of non-hydride molecules that have been/will be performed with ALMA, JVLA, the IRAM 30 m telescope, and APEX. There is a very strong synergy with theoretical models for H_2 formation within the turbulent ISM, several of which are under development by groups within our team. The possibility of now including hydride molecules within such simulations makes our proposed observing program very timely.

Anticipated results:

- A determination of the distribution function for the H_2 fraction in the Galaxy, and how it varies.
- A determination of the cosmic-ray ionization rate and how it varies
- An improved characterization of turbulence in the diffuse ISM, and its dissipation in regions of elevated temperature or ion-neutral drift.
- The provision of enhanced data products that will serve as a legacy for future ISM studies

SCIENTIFIC JUSTIFICATION

1. Introduction: Hydrides in the Diffuse Interstellar Medium of our Galaxy

Interstellar hydrides – that is, molecules containing a single heavy element atom with one or more hydrogen atoms – were among the first molecules detected outside the solar system. They lie at the root of interstellar chemistry, being among the first species to form in initially-atomic gas, along with molecular hydrogen and its associated ions. Because the chemical pathways leading to the formation of interstellar hydrides are relatively simple, the analysis of the observed abundances is moderately straightforward and provides ***key information about the environments where hydrides are found***.

Diffuse molecular clouds play a crucial role in the lifecycle of the interstellar medium, representing transitional objects that are intermediate between the diffuse atomic medium and the dense molecular clouds that are the sites of star formation. They provide a simple laboratory in which we can study a variety of physical and chemical processes of broad applicability in astrophysics. ***Because roughly one-half of the molecular material within the Galaxy is "CO-dark" (Grenier et al. 2005), small (diatomic and triatomic) hydrides are essential and often unique tracers of molecular gas in the diffuse ISM.*** Recent years have seen rapid progress in our understanding of interstellar hydrides, thanks largely to far-IR and submillimeter observations performed with the *Herschel Space Observatory,* the Atacama Pathfinder Experiment *(*APEX), and SOFIA. Knowing the exact state of – and distribution between – the various phases of the cold neutral medium (diffuse atomic gas, diffuse molecular gas, and dense molecular gas) ***will give crucial constraints on star-formation theories, by constraining the formation times of molecular gas out of atomic gas and shedding light on the life cycle of molecular clouds when they move between arm and interarm regions***. Indeed, understanding how molecular clouds form from the diffuse medium, and understanding the physical environment in which such clouds reside, are key goals of ISM physics. ***The survey of light hydrides proposed here is particularly timely, now that theoretical simulations of the ISM are starting to include chemistry, thereby allowing observations to be compared to specific model predictions for the first time.***

Observations that we have performed over the past decade using *Herschel/*HIFI*,* APEX, and SOFIA/GREAT have allowed the ground-state rotational transitions of several interstellar hydrides to be observed for the first time at high spectral resolution: these include OH (e.g. Wiesemeyer et al. 2016), OH^+, H_2O^+ (e.g. Wyrowski et al. 2010; Ossenkopf et al. 2010; Gerin et al. 2010a; Neufeld et al. 2010a; Indriolo et al. 2015), CH (e.g. Gerin et al. 2010b, Wiesemeyer et al.), CH^+(Falgarone et al. 2010), ArH^+ (Schilke et al. 2014), SH^+ (Menten et al. 2011), SH (Neufeld et al. 2012, 2015), HF (Neufeld et al. 2010b; Sonnentrucker et al. 2010), H_2Cl^+ (Lis et al. 2010; Neufeld et al. 2012), and HCl^+ (de Luca et al. 2012.) Because they possess small moments of inertia, hydrides typically have rotational transitions in the terahertz range ***where strong atmospheric absorption renders ground-based observations very difficult or impossible.*** These observations, carried out toward bright background continuum sources in the Galactic plane, revealed absorption in foreground clouds that intersect the sight-line to the observed continuum source; multiple absorbing clouds were frequently detected, with Doppler velocities that are nicely separated, both from each other and from the background continuum source, thanks to the differential rotation of the Galaxy.

Because the observed transitions all have high critical densities (i.e. densities at which the rates of collisional deexcitation equal the spontaneous radiative decay rate), most molecules are typically in the ground state within the diffuse ISM; thus, ***the absorption line strengths directly yield robust quantitative estimates of the molecular column densities in the foreground material, providing a particularly "clean" experiment.*** As we will discuss in Section 2 below, the careful analysis of hydride abundances obtained from *Herschel* observations have demonstrated the potential of absorption line studies of interstellar hydrides to probe the physical and chemical conditions in diffuse clouds, ***providing unique information***

about (1) the H_2 fraction within such clouds (and the importance of CO-dark gas), (2) the cosmic-ray ionization rate and (3) the effects of shocks and turbulent dissipation.

While previous *Herschel* observations of interstellar hydrides have been limited to a fairly small set of sight-lines almost entirely within the inner Galaxy, the 4GREAT instrument commissioned last year on SOFIA provides a ***unique and powerful tool for significantly expanding the set of observations available to probe the diffuse ISM throughout the Galaxy.*** As will be discussed in Section 3, ***4GREAT will be extremely efficient because of its capability of observing multiple hydrides in different spectral bands simultaneously***; this will allow simultaneous observations of five key hydrides (ArH^+, OH^+, H_2O^+, SH and OH) along with atomic oxygen using the GREAT High Frequency Array (HFA). Additional observations of C^+ and CH using the GREAT Low Frequency Array (LFA) will provide key information needed to fully exploit the 4GREAT observations.

2. Interstellar hydrides as diagnostic probes

2.1 The H_2 fraction in the interstellar gas, as probed by ArH^+, OH^+ and H_2O^+

While the neutral hydrides that we will observe (i.e. SH and CH) are most abundant in gas with a large molecular fraction, $f(H_2)$, several molecular ions show peak abundances in material with a smaller H_2 fraction. This behavior is particularly notable for ions that are destroyed rapidly by reaction with H_2: these include ArH^+, which is destroyed by proton transfer to H_2 (Schilke et al. 2014), and OH^+ and H_2O^+, which undergo H-atom abstraction reactions to form H_2O^+ and H_3O^+ respectively. ***The $n(OH^+)/n(H_2O^+)$ ratio is a particularly valuable probe of the H_2 fraction*** (Neufeld et al. 2010), because the reaction of H_2 with OH^+, which forms H_2O^+, competes with dissociative recombination of OH^+ with electrons (Figure 1); thus, the $n(OH^+)/n(H_2O^+)$ ratio is larger in regions of small $f(H_2)$ and smaller in regions of large $f(H_2)$.

The analysis of OH^+ and H_2O^+ absorption features, detected by Herschel along the sight-lines to bright Galactic continuum sources, ***revealed a substantial amount of interstellar gas with a molecular hydrogen fraction of a few percent*** (Indriolo et al. 2015). Of course, because the observations measure a ratio of column densities rather than volume density (i.e. $N(OH^+)/N(H_2O^+)$ rather than $n(OH^+)/n(H_2O^+)$), the $f(H_2)$ values thereby derived are really averages over the material that contributes most to the OH^+ and H_2O^+ absorption. These $f(H_2)$ values may therefore differ substantially from those derived for the entire sight-line from a comparison of $N(H_2)$ and $N(H)$. The argonium ion, ArH^+, traces material of even smaller $f(H_2)$. Because the dissociative recombination of ArH^+ is unusually slow, reactions with H_2 become the dominant destruction mechanism for $f(H_2) > 10^{-4}$ and the ArH^+ abundance starts to drop once $f(H_2)$ increases beyond that value. Thus, as discussed by Schilke et al. (2014), ***ArH^+ serves as a unique probe of material that is almost purely atomic***. This prediction for the behavior of ArH^+ is supported by the observational finding that the distribution of ArH^+ is entirely different from that of the other interstellar hydrides.

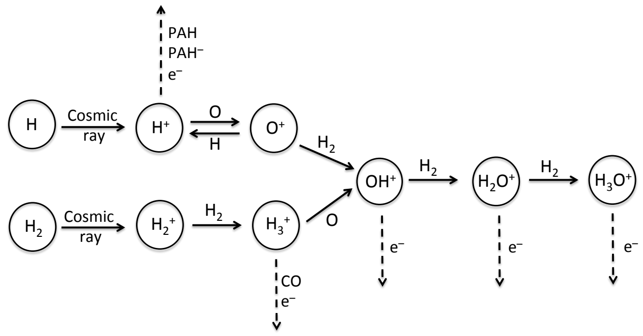

Figure 1: Chemical pathways leading to the oxygen hydride cations OH^+, H_2O^+ and H_3O^+. Dashed lines indicate competing reactions that reduce the abundance of these cations.

2.2 The cosmic-ray ionization rate in the diffuse ISM

In addition to providing valuable probes of the H_2 fraction in the Galactic ISM, the observed abundances of the molecular ions OH^+, H_2O^+, and ArH^+ allow the cosmic-ray ionization rate to be estimated. Because oxygen and argon have ionization potentials higher than that of hydrogen, both atoms are primarily neutral in the cold neutral medium; thus, the formation of hydride ions OH^+, H_2O^+, and ArH^+ is driven by cosmic-ray ionization (Gerin et al. 2010a; Neufeld et al. 2010a; Neufeld & Wolfire 2016). As shown in Figure 1, the formation of OH^+ and H_2O^+ occurs in a reaction sequence initiated by the cosmic-ray ionization of H (upper pathway) or H_2 (lower pathway). In the case of ArH^+, the formation pathway begins with the cosmic-ray ionization of Ar to produce Ar^+, which quickly reacts with H_2 to form ArH^+.

From a detailed analysis of the available *Herschel* data on OH^+, H_2O^+, and ArH^+, Neufeld & Wolfire (2017) obtained an estimate of the cosmic-ray ionization rate within diffuse ***atomic*** clouds (i.e. clouds with a molecular fraction of a few percent or less). The average value obtained for the primary ionization rate per H atom, $\zeta_p(H) = (2.2\pm0.3) \times 10^{-16}\ s^{-1}$, ***was in excellent agreement with entirely independent estimates*** of $\zeta_p(H)$ obtained for diffuse ***molecular*** clouds (with $f(H_2) > 0.1$) from observations of H_3^+. This value, however, is ***an order of magnitude larger than (1) the typical cosmic-ray ionization rates inferred for dense molecular clouds and (2) expectations based on direct measurements of cosmic-rays obtained with the Voyager I spacecraft.*** This suggests (1) that cosmic-rays are excluded from dense molecular clouds (e.g. Padovani et al. 2009); and (2) that the cosmic-ray flux in the vicinity of the solar system may be atypical.

2.3 A "warm chemistry" probed by SH

While OH^+, H_2O^+, and ArH^+ are produced by exothermic reaction sequences that are rapid at the temperatures (≤ 80 K) typical of the diffuse ISM, the formation of other hydrides – including CH^+, SH^+, and SH – can only take place by means of endothermic reactions driven by elevated temperatures or (in the case of SH^+ and CH^+) by ion-neutral drift. ***The abundances measured in the diffuse ISM for CH^+, SH^+, and now SH (thanks to SOFIA/GREAT), are all many orders of magnitude larger than the predictions for quiescent, cold clouds, suggesting that some fraction of the volume is occupied by a warmer phase*** heated by shocks and/or other processes that lead to the dissipation of interstellar turbulence (Godard et al. 2009; Godard et al. 2014; Neufeld et al. 2015).

3. Observations proposed here

Notwithstanding the insights obtained from previous observations of interstellar hydrides, the existing data have been acquired along a rather limited set of sight-lines, lying primarily in the first quadrant of the Galaxy and probing foreground gas situated almost exclusively in the inner Galaxy. In the legacy program proposed here, we will more than ***double the number of sight-lines along which the target hydrides have been observed***, and – equally important – ***our expanded sample will extend to regions within the Galaxy that were previously unexplored.*** Such an advance is now possible thanks to 4GREAT, which will allow five hydrides to be observed at the same time: OH^+, H_2O^+, ArH^+, SH, and OH. In addition to the observations of these five species, we will also observe C^+ and CH using the LFA with two separate local oscillator (LO) settings. These species are known to provide excellent tracers of the total column densities of H nuclei and H_2 (e.g. Sheffer et al. 2008) respectively, and will therefore provide the key information needed to convert the column densities measured for the other hydrides into *abundances* (relative to H_2 or H nuclei) that can be compared directly with interpretive models. When combined with observations of the HI 21 cm line, C^+ is also valuable in measuring the elemental carbon abundance.

All the 4GREAT and LFA observations will automatically be accompanied by simultaneous HFA observations of absorption by atomic oxygen. Together with the 4GREAT observations of OH, these measurements of O will provide additional anchor points for modeling the oxygen chemistry and also estimates of the elemental oxygen abundance. In Table 1, of the feasibility section, below, we list the set of eight transitions to be observed in the three setups that we will employ.

Our target list consists of 22 submillimeter continuum sources in the Galactic plane with 160 μm (1.9 THz) continuum fluxes in excess of 1000 Jy. As discussed in greater detail in the *Feasibility and Path to Publication* section, our total integration time of 1.6 hr per source (1.0 hr with 4GREAT and 0.6 hr with LFA) will provide a typical signal-to-noise ratio of > 50 on the continuum at all frequencies, providing a sensitive probe of foreground interstellar gas. The target sources, at estimated distances from the Sun ranging from 2 to 16 kpc are situated over a wide range of Galactic longitude. Five sources are in the outer Galaxy, at Galactocentric distances up to 10 kpc.

4. Analysis and exploitation of the data

The data obtained in this 72 hr legacy program will consist of absorption spectra obtained for 8 transitions toward 22 sources. Standard data reduction methods routinely implemented by the GREAT team have proven very successful in removing instrumental effects and correcting for telluric absorption, and our team has extensive experience in sideband deconvolution and the deconvolution of hyperfine structure. The resultant spectra will enable precision measurements of the column densities of the 8 target species in multiple diffuse clouds intersected by each sight-line. These column densities, and the abundance ratios they imply, will be interpreted using a wide range of theoretical tools.

These include (1) large grids of diffuse cloud models used previously to infer cosmic-ray ionization rates and molecular fractions from observations of ArH^+, OH^+, and H_2O^+ (Neufeld & Wolfire 2016, 2017); (2) models for sulphur chemistry in interstellar shocks and turbulent dissipation regions (TDRs; Godard et al. 2012; Neufeld et al. 2015); and (3) models for the formation of hydride molecules based on simulations (e.g. Bialy et al. 2017) of the H_2 fraction in the turbulent interstellar medium. The development of the latter is being carried out independently by three subgroups within our team (led by Valdivia, by Seifried and by Bialy). Figure 2 shows example simulations obtained by Seifried, in which the distribution of gas is shown separately for the "molecular phase" ($f(H_2) > 0.5$), "transition phase" ($f(H_2) = 0.05 – 0.5$) and "atomic phase" ($f(H_2) < 0.05$).

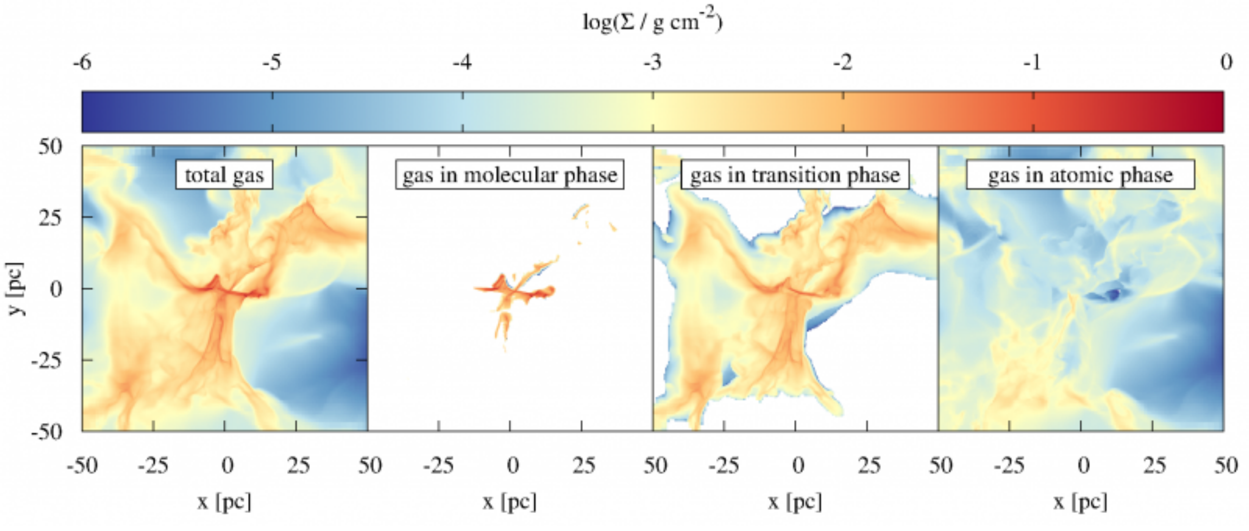

Figure 2: example results from an ISM simulation, showing the surface density of gas in the "molecular phase" ($f(H_2) > 0.5$), "transition phase" ($0.05 < f(H_2) < 0.5$) and "atomic phase" ($f(H_2) < 0.05$)

The expected results of the investigation will be:

- A determination of the distribution function for the H_2 fraction in the Galaxy, and how it varies (if at all) with position. By combining observations of ArH^+, OH^+, H_2O^+ and CH, we will determine the mass fraction of gas, dM, with H_2 fraction in the range $f(H_2)$ to $f(H_2) + df(H_2)$. This will be compared with models for the turbulent ISM to constrain key parameters that characterize the turbulence, such as the Mach number and the driving scale.
- A determination of the cosmic-ray ionization rate, and how it varies with position in the Galaxy and depth into a cloud. Here, we will probe systematic variations with Galactocentric radius and cloud column density, as well as random variations from one location to another. This determination will provide insight into the origins of low energy cosmic-rays within the Galaxy.
- An improved characterization of "warm chemistry" in the diffuse ISM, using measurements of SH, that will constrain models for shocks and turbulent dissipation regions.

5. Enhanced data products

We will provide a set of enhanced data products, consisting of tabulated column densities as a function of LSR velocity for all species observed toward all target sources, together with Gaussian fits to these column densities. These products will be a valuable legacy for future ISM studies, and will be published and made available at a permanent data repository such as CDS.

6. Ancillary data

Where necessary, we will propose to obtain the kinds of ancillary data that have proven useful in the interpretation of previous *Herschel* and SOFIA observations of hydrides. As a baseline for our abundance data, we will derive atomic hydrogen column densities from observations of the 21 cm radio line obtained with the NRAO K. G. Jansky Very Large Array (JVLA) and the Australia Telescope Compact Array (ATCA) for northern and southern sources, respectively. These will be acquired from the JVLA and ATCA archives or via newly-proposed observations with these instruments. We have already demonstrated our use of such data (obtained by Winkel et al. 2017) in the context of sources observed with *Herschel*. For the interpretation of SH, observations of additional sulphur-bearing molecules (CS, H_2S and SO_2) obtained with the IRAM 30 m telescope have proven very valuable (Neufeld et al. 2015). In addition, for sources where they have not already available, we will propose to acquire IRAM, APEX or ALMA spectra of additional species that may be observed from the ground: these include HCO^+, a valuable tracer of molecular hydrogen; SH^+, another key shock tracer; and atomic carbon.

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FEASIBILITY AND PATH TO PUBLICATION NARRATIVE

1. Line selection

Our selection of spectral lines has been chosen to maximize the scientific output using an efficiently-executed set of observations. The 8 transitions listed in Table 1, all originating in the ground-states of the target species, can be observed in just three spectral setups. The detectability and diagnostic value of all eight transitions have extensively demonstrated in observations performed with *Herschel*/HIFI or SOFIA/GREAT.

Table 1: List of target lines

Species	Transition	Frequency (GHz)	Setup	Receiver
H_2O^+	$1_{10} - 1_{01}$ $J = 3/2 - 3/2$	607.2258	#1	4GREAT CH1 LSB [a]
ArH^+	$J = 1 - 0$	617.5252	#1	4GREAT CH1 USB [a]
OH^+	$N_J = 1_2 - 0_1$	971.8038 [b]	#1	4GREAT CH2
SH	$^2\Pi_{3/2}$ $J = 5/2 - 3/2$	1382.9086 [b], 1383.2397 [b]	#1	4GREAT CH3
OH	$^2\Pi_{3/2}$ $J = 5/2^- - 3/2^+$	2514.3167 [b]	#1	4GREAT CH4
CH	$N_J = 2_{3/2^-} - 1_{1/2^+}$	2006.7991 [b]	#2a	LFA [c]
C^+	$^2P_{3/2} - {}^2P_{1/2}$	1900.5372	#2b	LFA [c]
O	$^3P_1 - {}^3P_2$	4744.7775	All	HFA

[a] LSB = “lower side band”; USB = “upper side band”

[b] Frequency of the strongest hyperfine component: additional components are at 971.8053 and 971.9192 GHz (OH^+); 1382.9041, 1382.9153, 1383.2350 and 1382.2463 GHz (SH); 2514.2987 and 2514.3532 GHz (OH); and 2006.7489 and 2006.7626 GHz (CH)

[c] We expect that the LFA can be re-tuned within a given flight leg to “hot switch” between settings 2a and 2b

Figure 3 shows example absorption spectra obtained from *Herschel*/HIFI and SOFIA/GREAT.

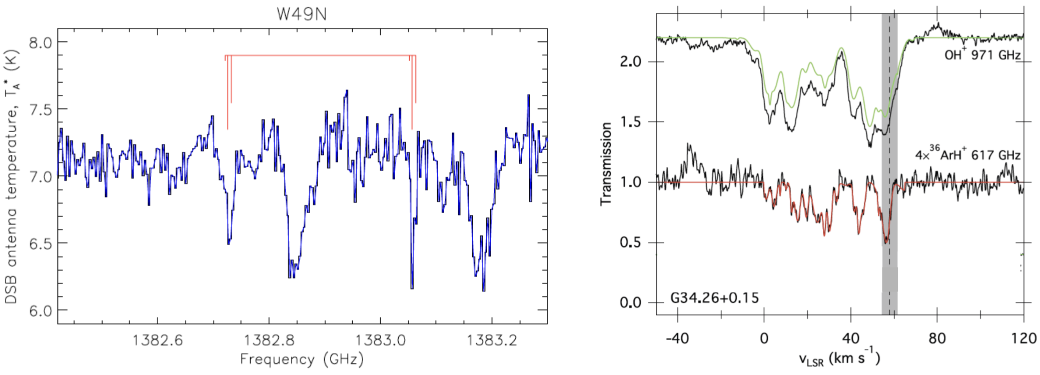

Figure 3: Example spectra for three of the target transitions. Left panel: discovery spectrum of SH, obtained with SOFIA/GREAT (Neufeld et al. 2012) toward W49N. The lambda doubling and hyperfine splittings are indicated by the red bars for a component at an LSR velocity of 40 km s^{-1}. Right panel: OH^+ and ArH^+ spectra obtained by *Herschel*/HIFI toward G34.26+0.15. For OH^+, the spectrum is shown before (black) and after hyperfine deconvolution (green). The ArH^+ spectrum is stretched by a factor of 4 in the vertical direction for clarity.

2. Source selection:

The goals of this proposal will be met by performing absorption-line spectroscopy of foreground interstellar gas along the sight-lines to bright background continuum sources. We require such sight-lines to intersect as many ISM structures as possible, including those in the outer Galaxy.

For a given column density, the signal-to-noise ratio obtained for an absorption feature is proportional to the continuum flux: thus, the most favorable sources are those possessing the largest continuum fluxes within the far-IR wavelength range (119 – 494 μm) encompassing our target lines. To identify suitable background sources, we used the source catalog of the Hi-GAL Galactic Plane survey, which provides continuum fluxes at 70, 160, 250, 350 and 500 μm. To maximize the amount of foreground material that can be traced by our observations, we imposed a minimum source distance of 5 kpc in the inner Galaxy and 2 kpc in the outer Galaxy, although many of the sources are at much larger distances. Here, we made use of kinematic distances that were recently estimated by the VIALACTEA team (Mège et al., in preparation), who extended the approach of Russeil et al. (2011 A&A, 526, 151) with an expanded set of spectroscopic surveys and with refined assignments of the most reliable radial velocity component.

From this source catalog, we selected sources in the inner Galaxy with 160 µm continuum fluxes exceeding 2000 Jy, corresponding to a brightness temperature of 2.7 K. (In some sources, the fluxes were above the saturation limit: here, the observations provided only lower limits on the flux, all of which were in excess of 2000 Jy.) For the outer Galaxy, we had to lower the flux threshold to 1000 Jy to obtain a sufficient number of target sources. The positions of the background sources were checked against known millimeter-wave sources, HII regions and masers using SIMBAD. Our list includes a few sources for which partial spectroscopic data is available from Herschel/HIFI – most often from the PRISMAS Key Program – but where the complete set of species available to 4GREAT has not yet been observed. In particular, because it was only late in the *Herschel* mission that the ArH^+ molecular ion was identified and its great value as a tracer recognized (Schilke 2014), the available dataset from *Herschel* is missing several determinations of the ArH^+ column density.

All of our sources are located in the Galactic plane, where *Herschel* observations have indicated that most of the volume is filled with a variety of diffuse gas components that will show up in one or more of our tracers, ensuring that we will detect line-of-sight absorption components toward all sources.

3. Observing times:

Observing times were estimated using the SOFIA Instrument Time Estimator (SITE). We adopted a typical source flux of 2000 Jy at 2 THz (150 µm), and the spectral shape computed for a typical dust temperature of 30 K and optical depth of 1.0 $(\nu/600\ \mathrm{GHz})^2$. For such a source, we require a signal-to-noise ratio of 50 on the continuum in a 1 km/s velocity bin, which allows an absorption feature with a depth of only 10% to be detected at the 5 sigma level in a 1 km/s wide bandpass. For the outer Galaxy, where our flux threshold is 1000 Jy, for some sources we will have to rebin the velocity resolution to 4 km/s in order to achieve a 5 sigma detection of a 10% absorption feature.

For these parameters, the 4GREAT observing time is dominated by the OH channel. While some of the target sources have a larger flux than that assumed (and a few have a smaller flux), our strategy is to spend the same time on each source and to accept a variable signal-to-noise ratio. In our experience with *Herschel*, we found that this strategy is superior to one in which the integration time is varied to provide a constant signal-to-noise ratio. (In practice, the latter strategy requires one to spend a large fraction of the available time on the very weakest sources, whereas the strategy we propose provides very high sensitivity to gas on sight-lines to strong sources at a moderate cost in observing time, and adequate sensitivity to probe the ISM on all sight-lines.)

We need 3 setups in total, one with 4GREAT to observe ArH^+/p-H_2O^+ (in the upper and lower sidebands respectively) in channel 1, OH^+ in channel 2, SH in channel 3 and OH in channel 4. When using the LFA, we will need 2 setups, one for C^+ and one for CH. The way GREAT is configured, the HFA will automatically be operational during all observations. Because of the limited simultaneous bandwidth available with the HFA, we will divide the observing time, as needed, between multiple LO settings to obtain the velocity coverage that is needed for each source when probing absorption by atomic oxygen.

4. Path to publication:

As explained below in the *Implementation Narrative*, we will perform a multi-tier analysis of data we obtain. The first stage (Task I, see the *Implementation Narrative* below) will entail the initial determination of column densities for all the eight target species. This analysis will draw heavily on techniques developed by the consortium members for Herschel/HIFI data analysis. These involve the fitting of even complex hyperfine patterns with multiple components, and the disentangling of any line emission from other species from the background source. These techniques are very mature, and have been applied and tested relative to each other in multiple publications, so we expect this stage of the data analysis, and the resulting publication, to be completed rapidly. At this stage we would also deliver an enhanced data product, consisting of column density tables for all sources and absorption components.

Similarly, in Task II, we will obtain simple estimates of the H_2 fraction and cosmic-ray ionization rate, relying on tried and true procedures and already existing model grids. This should result in a rapid publication. Task III, the comparison with simulations of the ISM, builds on ongoing efforts; here, we expect the time required to be somewhat longer. This is partly because including the chemistry of our target species and synthetic spectra is a fairly new development, and needs to be tested extensively. Another challenge will be to harmonize the results of the three different approaches by the three different theoretical groups working on this issue in the consortium, but once this is done, the result will be very robust.

Tasks IV (interpreting SH in the framework of simulations of shocks and TDRs), V (oxygen and carbon abundances), and VI (neutral hydrides), will rely on obtaining ancillary data, which will determine the timescale for publication. Conceptually, the techniques needed for these tasks, and the shock and TDR models, are available and tested, so no problems are expected.

BUDGET NARRATIVE

Salary support

Most of the funding requested is for salary support of four US investigators: Neufeld (25% FTE); one postdoc (100% FTE) who will be hired to work on this program for 2.5 years at Johns Hopkins under Neufeld's supervision; Wolfire (33.3% FTE); and Lis (13% FTE) The hourly rates listed in the proposal were computed for an assumed annual work time of 1950 hours, and are fully-burdened (i.e. include benefits ***and overheads***.) The overhead rates at JHU and UMd are 63.75% and 54.5% respectively. The duration of the period-of-performance is 3 years.

Travel

Funding is requested for each of these four US-funded investigators to make annual trips of duration 6 days to attend collaboration meetings in Cologne, Germany. These trips were costed using standard US State Department accommodation and ME&I rates, with airfare and car rental estimates from Expedia.

Other direct costs

Publications: We have budgeted for two 15-page ApJ papers and one 10-page ApJ paper in each of the three years of the project period.

BUDGET FORM

SOFIA Contract NNA17BF53C
Period of Performance: April 1, 2019 - March 30, 2022
Summary of Cost and Fee

			FY20 Oct 19 - Sep 20		**FY21 Oct 20 - Sep 21**		**FY22 Oct 21 - Sep 22**		**FY23 Oct 22 - Sep 23**	**Grand Total**	
Direct Labor Hours											
Name	**Labor Category**										
David A. Neufeld (Johns Hopkins)	Data analysis and interpretation		243.8		487.5		487.5		243.8	1,463	25% FTE
Postdoc TBD (Johns Hopkins)	Data analysis and interpretation		0.0		1,950.0		1,950.0		975.0	4,875	100% FTE
Darek Lis (JPL)	Data analysis and interpretation		127.0		254.0		254.0		127.0	762	13% FTE
Mark G. Wolfire (UMd)	Data analysis and interpretation		325.0		650.0		650.0		325.0	1,950	33.3% FTE
Sub- Total Labor Hours			695.8		3,341.5		3,341.5		1,670.8	9,050	
Direct Labor Costs (fully burdened w/o fee)		Note 1									
Name	**Labor Category**	**Rate**		**Rate**		**Rate**		**Rate**			
David A. Neufeld (Johns Hopkins)	Data analysis and interpretation	$222.75	$54,296	$229.43	$111,849	$ 236.32	$115,204	$ 243.41	$59,330	$340,679	
Postdoc TBD (Johns Hopkins)	Data analysis and interpretation	$73.64	$0	$75.85	$147,899	$ 78.12	$152,336	$ 80.46	$78,453	$378,689	
Darek Lis (JPL)	Data analysis and interpretation	$236.00	$29,972	$243.08	$61,742	$ 236.00	$59,944	$ 243.08	$30,871	$182,529	
Mark G. Wolfire (UMd)	Data analysis and interpretation	$122.81	$39,913	$126.49	$82,222	$ 130.29	$84,688	$ 134.20	$43,614	$250,438	
Sub- Total Labor Dollars			$124,181		$403,712		$412,173		$212,269	$1,152,336	
Travel	**Destination/Description**	**# Trips**		**# Trips**	Note 2	**# Trips**		**# Trips**			
Round Trip Airfare:	Baltimore/Washington or LAX - Cologne	0	$0	4	$4,400	4	$4,532	4	$4,668	$13,600	
Hotel:		0	$0	4	$5,856	4	$6,032	4	$6,213	$18,100	
ME&I:		0	$0	4	$3,416	4	$3,518	4	$3,624	$10,559	
Miscellaneous:		0	$0	4	$0	4	$0	4	$0	$0	
Local Transport:		0	$0	4	$300	4	$309	4	$318	$927	
Rental Car/Taxi/Other:		0	$0	4	$1,000	4	$1,030	4	$1,061	$3,091	
Burden on Travel	49.25% average		$0	4	$7,374	4	$7,595	4	$7,823	$22,791	
Sub-Total Travel Costs			**$0**		**$22,346**		**$23,016**		**$23,707**	$69,068	
Other Direct Costs (ODC's)											
Item	**Purpose/Description**										
Publications	40 journal pages in 3 articles / year		$0		$5,079		$5,231		$5,388	$15,699	
			$0		$0		$0		$0	$0	
			$0		$0		$0		$0	$0	
			$0		$0		$0		$0	$0	
			$0		$0		$0		$0	$0	
			$0		$0		$0		$0	$0	
			$0		$0		$0		$0	$0	
Burden on ODC's	63.75% IDC		$0		$3,512		$3,617		$3,726	$10,856	
Sub-Total ODC's			**$0**		**$8,591**		**$8,849**		**$9,114**	$26,554	
Total Cost			**$124,181**		**$434,649**		**$444,038**		**$245,090**	**$1,247,958**	

Note 1: the labor costs listed include indirect costs as appropriate with each institution, following the instructions in CfP
Note 2: 4 trips per year means one trip per year for 4 people

IMPLEMENTATION NARRATIVE

The overall management and direction of the program will be led by **David Neufeld**, the non-German Co-PI, and **Peter Schilke**, the German Co-PI. Following the instructions given in the Call for Proposals (CfP), the non-German PI (Neufeld) has been designated as the formal PI; however, Neufeld and Schilke will share the task of directing the program equally, as Co-PIs.

Given the magnitude and legacy value of the set of data to be obtained in this program, we will undertake a vigorous program of analysis and interpretation that is supported by an intensive theoretical effort. We have convened a diverse team of 23 investigators from 5 countries to provide the extensive expertise that will be needed to exploit the data fully.

The data reduction, analysis, and interpretation will be organized into several tasks:

I. Initial data reduction and analysis: This first phase of analysis will yield column densities and relative abundances for each of the eight target species. It will be led by **Neufeld**, in collaboration with Schilke, Gerin, Lis, Sonnentrucker, Higgins and Indriolo, all of whom have extensive experience in the analysis of similar spectroscopic data from *Herschel*. Between them, they have led (i.e. as first author) more than two dozen journal articles presenting new high-resolution spectroscopic data from Herschel/HIFI and SOFIA/GREAT. Higgins is a member of the GREAT instrument team, and will contribute his extensive expertise on the data reduction side. In this task, we will analyse not only the mean abundances, but also the variances and co-variances of the measured abundances, and will use Principal Component Analysis to quantify and visualize the similarities and differences in the distribution of the various species (e.g. Neufeld et al. 2015).

II. Estimates of the H_2 fraction and the cosmic-ray ionization rate: Here, we will make use of an extensive grid of diffuse clouds models already in hand to obtain initial estimates of the H_2 fraction and cosmic-ray ionization rate in each absorbing cloud, using the methods discussed in Neufeld & Wolfire (2016, 2017). The variation of the H_2 fraction and cosmic-ray ionization rate with such parameters as cloud column density and Galactocentric radius will be investigated. This task will be led by **Wolfire**, with assistance with Indriolo and Neufeld, all of whom have extensive experience in this type of analysis.

III. Comparison with simulations of the turbulent ISM: In this phase of the analysis, we will confront the observations of the molecular ions with predictions obtained from hydrodynamical simulations of the turbulent ISM. Such simulations already include the chemical processes (H_2 photodissociation and grain-catalysed H_2 formation) needed to model the H_2 fraction (e.g. Bialy et al. 2017; see also Figure 2 in the Scientific Justification). They are being modified to include three key tracers of the molecular fraction: ArH^+, OH^+ and H_2O^+. Our program includes three teams who are working independently to incorporate oxygen and argon chemistry into the theoretical models: (1) the Köln team (Seifried, Walch, Schilke, Ossenkopf, Sanchez-Monge); (2) the Paris/Rome team (Valdivia, Gerin, Godard, Falgarone, Hennebelle, Elia and Molinari) and (3) the US/Israeli team (Bialy, Sternberg, Neufeld, and Wolfire). The redundancy in these cutting-edge theoretical activities will facilitate careful inter-comparisons to investigate their reliability. **Schilke** will be the task leader for this effort.

IV. Comparison with simulations of shocks and turbulent dissipation regions (TDRs): This task will be undertaken by Godard and Falgarone, who have pioneered the study of TDRs with G. Pineau des Forets. The analysis methods described recently in Neufeld et al. (2015) will be used and extended to interpret the SH spectra obtained in this program. The analysis of the SH abundance measurements, along with ancillary ground-based data to be acquired for other sulphur species (e.g. CS and H_2S), will allow the nature of the TDRs (ion-neutral velocity shifts) or shocks (shock velocities) to be elucidated. **Falgarone** will be the team leader for this task.

V. Oxygen and carbon abundances (from O and C^+): We will use our observations of C^+ and atomic oxygen to allow Galactic variations in the elemental abundances of C and O to be estimated. In addition to their intrinsic interest, such variations must be understood to facilitate the other tasks identified above. This effort will be led by **Gerin** and **Wiesemeyer**, in collaboration with Lis.

VI. Neutral hydrides (OH and CH) and ancillary data: the column densities of CH and OH will be used to estimate the total molecular hydrogen column density and further constrain the oxygen chemistry. The analysis will be led by **Wyrowski**, in collaboration with Menten, Wiesemeyer, Sanchez-Monge, and Sonnentrucker. Menten will contribute the HI data analysis.

Steering committee

The leads for these six tasks (Neufeld, Wolfire, Schilke, Falgarone, Gerin and Wyrowski) will constitute a steering committee that will conduct monthly or biweekly telecons, as needed, to ensure that the investigation is proceeding as planned. This committee consists of two team members at US institutions, two at German institutions, and two at non-German non-US institutions.

Fractional commitments of funded US-funded investigators

Our budget requests salary support for Neufeld, Wolfire and Lis at the 25%, 33.3%, and 13% levels for three years. We propose also to support one postdoctoral fellow at JHU to work 100% on this program. Depending upon the applicant pool, this postdoctoral fellow might work “closer to the data” (focusing on Tasks I and II above), or on the more theoretically-oriented tasks (Tasks III and IV).

Fractional commitments of non-US investigators

The Co-PI Schilke will commit 20-25% FTE to this program throughout its 3-year duration. For the other Co-I’s for whom funding is *not* requested in this proposal, the typical time commitment is 5 – 15% FTE. In some cases, the exact time commitment for these Co-I’s will be determined by the success of proposals for funding that will be submitted to European and national funding agencies should this joint legacy proposal be approved.

Publication strategy

We expect each of the six tasks enumerated above to lead to one or more substantial publications. In addition, there will likely be several additional papers describing the theoretical tools that are being developed for the program (particularly from the various teams working on Tasks III and IV above).

INVESTIGATOR BIOGRAPHICAL AND PUBLICATION DATA

David Neufeld (US Co-PI, PRINCIPAL INVESTIGATOR)

Prof. David Neufeld is a professor in the department of Physics and Astronomy at the Johns Hopkins University. His primary research interests are molecular astrophysics, astrochemistry, and infrared and submillimeter astronomy. His relevant experience includes being a Co-I on the Submillimeter Wave Astronomy Satellite (SWAS); an astronomy Co-I on *Herschel*/HIFI; a member of the SOFIA/EXES science team; a Co-I on several *Herschel* Key Programs including PRISMAS and HEXOS; and the PI on several *ISO, Spitzer, Herschel* and SOFIA programs. His recent research activities have emphasized observations of small interstellar molecules, particularly hydrides in diffuse clouds. Carefully interpreted with the use of astrophysical models, such observations provide unique information of broad astrophysical interest.

Relevant publications

“The Cosmic-Ray Ionization Rate in the Galactic Disk, as Determined from Observations of Molecular Ions,” Neufeld, D. A., & Wolfire, M. G., ApJ, 845, 163 (2017)

“SOFIA/GREAT Discovery of Terahertz Water Masers,” Neufeld, D. A., Melnick, G. J., Kaufman, M. J., et al., ApJ, 843, 163 (2017)

"The Chemistry of Interstellar Argonium and Other Probes of the Molecular Fraction in Diffuse Clouds," Neufeld, D. A. & Wolfire, M. G., ApJ, 826, 183 (2016)

"Interstellar Hydrides," Gerin, M., Neufeld, D. A., & Goicoechea, J. R., ARAA, 54, 181 (2016)

"Sulphur-bearing molecules in diffuse molecular clouds: new results from SOFIA/GREAT and the IRAM 30 m telescope, "Neufeld, D. A., Godard, B., Gerin, M., et al., A&A, 577, A49 (2015)

"Herschel Observations of Interstellar Chloronium. II. Detections toward G29.96-0.02, W49N, W51, and W3(OH), and Determinations of the Ortho-to-Para and ^{35}Cl/^{37}Cl Isotopic Ratios,"
Neufeld, D. A., Black, J. H., Gerin, M., et al. ApJ, 807, 54 (2015)

"Ubiquitous argonium (ArH^+) in the diffuse interstellar medium: A molecular tracer of almost purely atomic gas,” Schilke, P., Neufeld, D. A., Müller, H. S. P. et al., A&A, 566, A29 (2014)

"Discovery of interstellar mercapto radicals (SH) with the GREAT instrument on SOFIA,"
Neufeld D. A**.**, Falgarone, E., Gerin, M., et al., A&A, 542, L6 (2012)

"Herschel/HIFI observations of interstellar OH^+ and H_2O^+ towards W49N: a probe of diffuse clouds with a small molecular fraction, " Neufeld, D. A., Goicoechea, J. R., Sonnentrucker, P., et al., A&A, 521, L10 (2010)

"Strong absorption by interstellar hydrogen fluoride: Herschel/HIFI observations of the sight-line to W31C," Neufeld, D. A., Sonnentrucker, P., Phillips, T. G. et al., A&A, 518, L108 (2010)

Peter Schilke (German Co-PI)

Prof. Dr. Peter Schilke is a professor of astrophysics at the University of Cologne. He is an expert on star formation and astrochemistry. He uses predominantly high-resolution mm, submm and far-IR spectroscopy of the interstellar medium and star-forming regions, but is also involved in astrochemical modeling. The current efforts in this direction concern post-processing of MHD simulations with a chemical code his group has developed to obtain synthetic spectra. He was leader of the SgrB2(M) subproject of the Herschel/HIFI HEXOS key project, and has published a number of analyses of spectra similar to the ones anticipated in this program. The most remarkable of these was the detection of ArH^+ absorption in the ISM. He has developed fitting routines to deal with complex molecular spectra, which resulted in the publicly available XCLASS package that can perform automatic fits of complex spectra. He will be the German co-PI of this proposal, be involved in the data analysis aspects, and lead the comparison with simulations of the ISM

Shmuel Bialy (Co-I)

Dr. Shmuel Bialy is an ITC postdoctoral Fellow at the Harvard-Smithsonian Center for Astrophysics. Bialy works on various theoretical problems related to the structure and chemistry of the interstellar medium (ISM) in the Galaxy and in external galaxies. In his work, Bialy combines chemical (semi)-analytic modeling and high resolution magnetohydrodynamic (MHD) simulations to study the turbulent diffuse and dense interstellar phases, and the atomic-to-molecular (HI-to-H_2) transition. His recent work on the HI-to-H_2 transition in a turbulent medium (Bialy, Burkhart & Sternberg 2017) would serve a basis for the proposed study of the H_2 distribution using the ArH^+, OH^+, and H_2O^+ probes (see Scientific Justification, sections 2.1 and 4).

Davide Elia (Co-I)

Dr. Davide Elia is a staff researcher at the Institute for Space Astrophysics and Planetology (IAPS) in Rome (Italy), a structure within the Italian National Institute for Astrophysics (INAF). His research focuses on the observational study of the interstellar medium and star formation in the Milky Way. His main interest is in understanding the various stages of star formation, especially the early ones, with particular attention to the high-mass regime. In recent years, he has been deeply involved in the main observational programs of *Herschel* for star formation. He is member of large international consortia working on the main *Herschel* photometric large surveys *Hi-GAL*, *Gould Belt Survey*, and *HOBYS*, all aimed at observing the cold dust contained in the Galactic molecular clouds in the wavelength range where its thermal emission is expected to peak. In particular, he had the responsibility of compiling and publishing a catalog of the physical properties of the *Hi-GAL* compact sources. At the same time, he is involved in spectroscopic surveys of the interstellar medium on the Galactic plane, such as the CO mapping of the Vela-D cloud (with SEST) and the Forgotten Quadrant Survey project for observing large areas of the third Galactic quadrant with ARO. For the HyGAL project, he actively participated in the target list definition, by selecting *Herschel* sources with strong emission (or even saturated) at 160 micron. He will be involved in the comparison of the observations of molecular ions with simulations of the turbulent ISM.

Edith Falgarone (Co-I):

Dr. Edith Falgarone (Emeritus Director of Research, CNRS) is an expert on the physics of the interstellar medium (ISM) and star formation, with a particular emphasis on turbulence and magnetic fields. She has broad experience in millimeter and sub-millimeter molecular line observations. She has a decades-long expertise in leading many original studies to disclose the signatures of the intermittency of cosmic turbulence, its impact on the physics of the ISM and on star-formation. She was part of the *Herschel*/HIFI consortium and joined the Planck collaboration for the analyses of the Galactic foregrounds. She is leading the ALMA project on the CH^+ observations of redshifted starburst galaxies. She has been recently awarded an Advanced Grant of the European Research Council.

Maryvonne Gerin (Co-I):

Prof. Maryvonne Gerin is a senior scientist at CNRS. Her research interests are the study of the structure, dynamics and chemistry of interstellar clouds, from the diffuse clouds to the cold prestellar cores, and how these conditions are related to the star formation activity. As a Co-I for the HIFI instrument on board the *Herschel* satellite, she has led the PRISMAS Key Program dedicated to absorption spectroscopy of hydrides and ionized carbon. Follow-up work has been carried out with ALMA to calibrate the constancy of the abundance relative to H_2 of selected hydrides (CH, HF) and abundant molecules accessible from the ground. She has been involved in the French interdisciplinary programme PCMI, fostering collaboration between astrophysics, physics and chemistry, which triggered fundamental work on hydride reactivity and collisional excitation. She will contribute to the analysis and interpretation, and put a particular focus on the O and C^+ data as a means to track the Galactic gradient in the elemental carbon and oxygen abundances.

Benjamin Godard (Co-I):

Dr. Benjamin Godard is an astronomer of the Paris Observatory who specializes in the modeling of out-of-equilibrium chemistry, dynamics, and radiative transfer in turbulent dissipation regions (TDR), molecular shocks, photodissociation regions (PDR), X-ray dominated regions (XDR), and, more broadly, in the multiphase interstellar medium. Instigator of the TDR model, he is currently one of the main developers of the Meudon PXDR code, of the Paris-Durham shock code, and of a stand-alone numerical tool capable of post-processing the chemistry in 3D numerical simulations of interstellar turbulence obtained with the RAMSES MHD code. His task, in this project, will be to interpret the observations of the tracers of warm chemistry and the distribution and line profiles of the tracers of atomic and molecular gas. This will be done using the framework of state-of-the-art 1D chemical models but also via the developments of the chemical modeling of the 3D multiphase and turbulent ISM recently performed by Elena Bellomi, a PhD student at the Paris Observatory.

Patrick Hennebelle (Co-I):

Dr. Patrick Hennebelle is an expert of the dynamics of the interstellar medium and the star formation process. He performs heavy numerical simulations with adaptive mesh refinement codes on massively parallel super computers. He collaborates with observers to compare the results of these simulations with observational data.

Ronan Higgins (Co-I):

Dr. Ronan Higgins is a post doctoral researcher at the University of Cologne. He previously worked as a calibration scientist on the Herschel/HIFI instrument where he played a leading role determining the instrument response and resolving instrument data quality issues. He has also flown multiple times on SOFIA where his main roles are the upGREAT data calibration and observing support. He has recently led the observing and reduction of the largest velocity resolved [CII] map taken to date of the Orion A region. He is an expert in heterodyne instrument calibration effects.

Nick Indriolo (Co-I):

Dr. Nick Indriolo is currently a support scientist working at Space Telescope Science Institute. He has extensive research experience working with high spectral resolution, high signal-to-noise ratio observations targeting molecular absorption lines from near IR to sub-mm wavelengths. In particular, Nick is an expert in the use of molecular abundances to constrain cosmic-ray ionization rates in the interstellar medium. This makes him well-suited for both the analysis and interpretation of observations planned within this program. Additionally, by working at the intersection of two fields (astrochemistry and cosmic-ray physics), Nick is highly experienced in presenting results to scientific communities with very different backgrounds, and in fostering interdisciplinary collaborations.

Darek Lis (Co-I):

Dr. Darek Lis has 30 years of experience in the field of far-infrared/millimeter astrophysics. His research interests include high-resolution molecular spectroscopy of the interstellar medium and the solar system objects. He has been closely involved in observations of hydrides using ground-based and space-borne submillimeter facilities, including the Caltech Submillimeter Observatory and *Herschel*. He participated in the commissioning (July 2017) and early science observations using 4GREAT (December 2018), and will be involved in the data analysis and interpretation aspects of the SOFIA program.

Karl Menten (Co-I):

Prof. Karl M. Menten is the director for Millimeter and Submillimeter Astronomy at the Max Planck-Institut for Radio Astronomy (MPIfR) and the principal investigator of the Atacama Pathfinder Experiment (APEX). He has 35+ years of experience in radio and (sub)millimeter wavelength observations. His group at the MPIfR has conducted various large scale surveys with the APEX. These cover various CO transitions, providing complementary molecular line data. He presently supervises second year doctoral student Arshia Jacob whose dissertation centers on far-infrared and complementary radio wavelength observations of the CH radical.

Sergio Molinari (Co-I)

Dr. Sergio Molinari is a senior researcher at INAF (Instituto Nazionale di Astrofisica) in Rome and expert in Galactic star formation, with particular emphasis on global studies carried out with large scale Galactic Plane surveys. He has been PI of the Herschel/Hi-GAL open time Key-Project for the complete Plane survey between 70 and 500 micron with the *Herschel* satellite. Dr. Molinari was also PI of the FP7 EU-funded program VIALACTEA for the characterization of global star formation in the Milky Way, assembling major photometric and spectroscopic surveys from the near-infrared to the radio, and producing a catalogue of more than 150,000 dense clumps in the Galaxy with distances and physical parameters.

Volker Ossenkopf-Okada (Co-I):

Dr. Volker Ossenkopf-Okada is an expert in PDR modeling and in the analysis of the turbulent structure of the ISM, as well as an experienced GREAT observer. He is head of the Cologne PDR group, and PI of the project ``Modeling of Irradiated Molecular Clouds'' within the DFG-funded Collobarative Research Center SFB 956 in Cologne. He was PI of the *Herschel* key project on PDRs (WADI), which undertook observations of numerous PDRs. He will contribute to the analysis of the lines of C^+, OI, and the hydrides by including them in turbulent and PDR models, comparing the model output with the line observations and deriving best fitting model parameters.

Alvaro Sanchez-Monge (Co-I):

Dr. Alvaro Sanchez-Monge is a post-doctoral researcher at the University of Cologne. He is an expert in radio and (sub)millimeter observations and has strong expertise in the processing and reduction of spectral line data taken with a variety of astronomical facilities. He has been the PI of several observational projects using ALMA, JVLA, APEX, and IRAM 30m, and contributed to the analysis of spectral line observations of telescopes such as *Herschel* and SOFIA. He will be involved in the initial data reduction and analysis, and contribute to the analysis of the ancillary spectroscopic data.

Daniel Seifried (Co-I):

Dr. Daniel Seifried is a postdoctoral researcher in the working group of Prof. S. Walch at the Physical Institute at the University of Cologne. He is an expert on (magneto-) hydrodynamical simulations of star formation including the formation of molecular clouds out of the diffuse ISM. He also has great expertise in implementing and applying astrochemical networks in such simulations and is working on making detailed comparisons between simulations and observations. In this context, he will support the proposed project by participating in Task III.

Amiel Sternberg (Co-I):

Prof. Amiel Sternberg is a theoretical astrophysicist working in the fields of interstellar medium, astrochemistry, galaxy evolution, star formation, cosmic structure, black holes and active galaxies, plasma astrophysics, dynamics, spectroscopy and radiative transfer, computational methods and theory of fundamental processes. Sternberg is Yuval-Ne’eman Professor of Theoretical Physics at Tel Aviv University (TAU) in Israel, where he is a faculty member in the astronomy department, and serves as director of the Raymond and Beverly Sackler TAU-Harvard/ITC Astronomy Program. He is also senior associate scientist in the Garching Infrared Group at the Max-Planck-Institute for Extraterrestrial Physics in Germany, and is a Research Scientist at the Center for Computational Astrophysics, Flatiron Institute in New York City.

Paule Sonnentrucker (Co-I):

Dr. Paule Sonnentrucker is an ESA staff astronomer at STScI. Her expertise and research focus on using multi-wavelength spectroscopy to study the atomic and molecular species that define the Interstellar Medium (ISM) with a particular emphasis on understanding the physical and chemical processes at play in diffuse molecular and star-forming regions. She will participate in all aspects of the proposed in this work, from the data analysis using well-known, robust and extensively-tested methods to the interpretation of those results when compared to the state-of-the-art models described in this proposal.

Valeska Valdivia (Co-I):

Dr. Valeska Valdivia is an astrophysicist with particular experience in studying the physics of the interstellar medium (ISM) and the star formation process. She obtained her PhD at the Pierre et Marie Curie University, where she worked in the Radio-Astronomy Laboratory of the École Normale Supérieure. After her PhD, she was hired as a postdoctoral fellow at the Astrophysics Service of the CEA Saclay, working on the MAGMIST project and then the MagneticYSOs project, running and analysing high-resolution numerical simulations of the formation of molecular clouds and the formation of proto-stellar systems. As a result, she has a very strong background in high-performance computing, with extensive experience of coding new features into the adaptive mesh refinement code RAMSES. In particular, she has developed and optimized an innovative scheme for estimating column densities, and thereby computing shielding effects due to the attenuation of high-energy radiation, in numerical simulations of self-gravitating hydrodynamics. She has also introduced other features, including heating by cosmic rays, the formation, destruction and advection of molecular hydrogen and its thermal feedback on the gas. Dr. Valdivia has also developed the computational machinery to couple an extensive chemical solver to a post-processing tool; this allows her to study the influence of the dynamically calculated H_2 fraction on the other chemical abundances. She is currently a member of the MagneticYSOs ERC team, dedicated to studying the role of the magnetic field in the early phases of the star formation process; in this capacity she has been responsible for analysing numerical simulations of young stellar objects and for producing synthetic observations of polarized emission from dust.

Stefanie Walch-Gassner (Co-I):

Prof. Dr. Stefanie Karoline Walch-Gassner (neé Walch; hereafter SW) is a tenured, full professor for theoretical astrophysics at University of Cologne since 11/2013. She won an ERC Starting Grant in 2016 and is the PI of sub-project C5 “Star formation and feedback in molecular clouds” within the Collaborative Research Center 956 “Conditions and impact of star formation”, which is funded by the German Science Foundation (DFG). For example, she is an editor of Astronomy & Computing (ASCOM, Elsevier), is a member of the Academic Advisory Board of the University of Cologne, and an advisory board member of the extraterrestrial science program of the German Aerospace Center (DLR). SW has a track record of simulating the turbulent ISM, star formation and stellar feedback. Her current working group as of 09/2018 is composed of 5 postdocs, 4 PhD students, 6 MSc., and 2 BSc. students. Therefore, she will work on theoretically interpreting the HyGal observational data, which will be done by comparing the observations with state-of-the-art, high resolution simulations of molecular cloud formation and evolution carried out in the SILCC project (www.astro.uni-koeln.de/silcc).

Helmut Wiesemeyer (Co-I):

Helmut Wiesemeyer is a staff scientist at the mm and submm astronomy department of the Max Planck Institute for Radio Astronomy. His research interests comprise the chemistry of the ISM, stellar evolution, polarimetry and radiative transfer. As SOFIA scientist, he participated in about 100 science flights, has extensive experience with calibration and data reduction matters, and led or co-authored 33 peer-reviewed publications based on data from the GREAT instrument suite. Wiesemeyer's publication record includes several papers on the spectroscopy and chemistry of light hydrides in the ISM and in envelopes around star-forming regions.

Mark Wolfire (Co-I):

Dr. Mark Wolfire is a Principal Research Scientist in the Astronomy Department at the University of Maryland. He is an expert in modeling the chemistry and thermal structure of diffuse clouds and photodissociation regions (PDRs). His models have been used extensively to interpret infrared absorption line observations of the diffuse interstellar medium (Herschel) and infrared line emission from Galactic PDRs (KAO, *ISO, Spitzer*, SOFIA) and from the ISM of normal and starburst galaxies (KAO, *ISO, Spitzer, Herschel*). He will provide theoretical support for the analysis and interpretation of the data, in particular for estimates of the H_2 fraction and cosmic-ray ionization rate and for the comparison to simulations of the turbulent ISM.

Friedrich Wyrowski (Co-I):

Dr. Friedrich WyrowskI is a staff astronomer in the Submillimeter Astronomy group at MPIfR Bonn. His main research interests are massive star formation, the interaction of young massive stars with their environment, and the physical conditions in molecular envelopes around late type stars. His expertise includes high angular resolution studies using centimeter to (sub)millimeter interferometers, and he has extensive experience in submillimeter astronomy as the MPIfR project scientist for the APEX telescope. His has been the PI of several SOFIA projects focusing on NH_3 absorption studies.