Rationale for DD-ERS Program

> *"Observations with HST have confirmed that most nearby galaxies harbor supermassive black holes in their nuclei. How do these supermassive black holes form and evolve? Do they grow from stellar seeds or do they originate at the very beginning of the formation of a galaxy? These key questions are ripe for a frontal attack now. Addressing them will require the observation of active galactic nuclei (AGNs) when they first turn on, over the entire electromagnetic spectrum. With its enormous sensitivity in the infrared, NGST will be able to detect AGNs out to redshifts beyond 10."*
> – Astronomy and Astrophysics in the New Millennium (2000-2010 Decadal Survey).

Over 50 years after their formal identification, and over two decades since the calculation of their space density evolution, several fundamental facts remain unknown for high-luminosity AGN, i.e. quasars:
What is the main AGN triggering mechanism at the height of quasar activity at redshifts $z = 2 - 3$?
What is the direct, observational evidence in individual objects, that links AGN activity to star formation?
Can we observe "AGN feedback" in action, in situ for the most luminous sources at their peak activity?

These remain the outstanding observational extragalactic questions of our time. And they will be answered with the launch of the *James Webb Space Telescope*.

We propose the perfect Directors Discretionary Early Release Science (DD ERS) program. We have identified a population of infrared (20-30μm observed) bright quasars at the peak of cosmological quasar activity, $z \approx 2.5$. Their global star-formation properites are currently unknown, but observations with JWST MIRI, in particular MRS spectroscopy, will quantify the level of star-formation in these objects. Moreover, the IFU aspect of the Medium Resolution Spectrometer will allow, for the first time, detailed investigations of the both the central AGN IR emission and potentially extended emission.

The recently identified Extremely Red Quasar (ERQ) objects are a unique obscured quasar population with extreme physical conditions related to powerful outflows across the line-forming regions. These objects are found at the same cosmological epoch as the peak of quasar activity, $z \approx 2.5$ and are the best candidates to date to show outflows on galactic scales; we are seeing quasar-level AGN feedback in action, in situ.

With our ERS MIRI observations of these ERQ, so called since they are bright in the WISE W4 23μm band, we will deliver all the tools necessary to the community in order to optimize Cycle 2 proposals of 5-30μm milliJansky bright sources. This is *a fundamental tool* for the exploitation of a key MIRI instrument mode.
We will satisfy the Goals and Principles of the DD ERS program by:

- ensuring open access to our datasets in support of the preparation of Cycle 2 proposals, and
- engaging a broad cross-section of the astronomical community, in particular the extragalactic community, in familiarizing themselves with JWST data and scientific capabilities.

In particular, we aim to produce several key science products:

- `mrs_analyzer` A Python module for analyzing MRS data;
- `mrsfringe` A Python module for mitigating MRS fringing issues;
- a suite of science results on quasar feedback and evolution.

Critically, we have already begun working closely with the MIRI team (due to the P.I.'s location at Edinburgh) and will continue to develop tools here for the MIRI Imager and MRS.

The DD ERS program is guided by the following key principles:

- Projects must be substantive science demonstration programs that utilize key instrument modes to provide representative scientific datasets of broad interest to researchers in major astrophysical sub-disciplines. Note that a meritorious DD ERS project need not cover every mode of the observatory. The request should match the focused science goals of the proposal.
- Projects must design, create, and deliver science-enabling products to help the community understand JWST's capabilities. An initial set of products must be delivered by the release of the Cycle 2 GO Call for Proposals (September 2019). Each project must define a core team to be responsible for the timely delivery of such products according to a proposed project management plan, with performance subject to periodic review.
- All observations must be schedulable within the first 5 months of Cycle 1 (planned to be from April to August 2019), and a substantive subset of the observations must be schedulable within the first three months. Target lists must be flexible to accommodate possible changes to the scheduled start of science observations.
- Both raw and pipeline-processed data will enter the public domain immediately after processing and validation at STScI. These data will have no exclusive access periods (i.e., no proprietary time).

STScI recognizes and supports the benefits of having diverse and inclusive scientific teams involved in the formulation of ERS proposals. Programs with diverse representation of community members in a given sub-discipline helps ensure that the investigations will be of broad interest. Broad involvement also facilitates the dissemination of JWST expertise through a more extensive network, and promotes more equitable participation in JWST scientific discovery.

The DD ERS program will be essential for informing the scientific and technical preparation of Cycle 2 General Observer (GO) proposals, submitted seven months after the end of commissioning.

The Medium-Resolution Spectrometer: The JWST MIRI medium-resolution spectrometer (MRS; Wells et al. 2015) will observe simultaneous spatial and spectral information between 4.9 and 28.8 μm over a contiguous field of view up to 7.2” 7.9” in size. This is the only JWST configuration offering medium-resolution spectroscopy (with R from 1500 to 3500) longward of 5.2 μm.

MRS observations are carried out using a set of 4 integral field units (IFUs), each of which covers a different portion of the MIRI wavelength range. MRS IFUs split the field of view into spatial slices, each of which produces a separate dispersed ”long-slit” spectrum. Post-processing produces a composite 3-dimensional (2 spatial and one spectral dimension) data cube combining the information from each of these spatial slices. This process is illustrated schematically in Figure 1. MRS operations have been designed to allow for efficient observations of point sources, compact sources, and fully extended sources. The observer will have control over 3 primary variables: (1) wavelength coverage, (2) dithering pattern, and (3) detector read out mode and exposure time (via the number of frames and integrations).

Relation to Spitzer IRS:
Major Achievement of Spitzer was IRS.
However IRS had fringing.
Also, Spitzer IRS died before WISE; therefore now WISE W4 objects were observed by the IRS.

■ Scientific Justification

One lasting scientific legacy of the *Hubble Space Telescope (HST)* will be the discovery of giant black holes at the centers of galaxies, confirming the longstanding theory of the "central engines" of quasars. One of the major surprises from the *Hubble* was the discovery of a correlation between black hole mass and galaxy properties. This connection, causal or otherwise, may provide crucial clues to how and why these black holes formed and how their host galaxies evolved. *As of the launch of the James Webb Space Telescope (JWST), this is one of the outstanding questions in astrophysics.*

Furthermore, discovery of spectral lines in active galaxies reveals that black holes can trigger massive star formation. As such, The link between massive galaxies and the central super-massive black holes (SMBHs) that seem ubiquitous in them is now thought to be vital to the understanding of galaxy formation and evolution ([1], [2]), and huge observational and theoretical effort has been invested in trying to measure and understand the physics involved in these enigmatic systems. The two main energy sources available to a galaxy are nuclear fusion in stars and gravitational accretion onto compact objects, and we still do not fully understnad the interaction of an active galactic nuclei and the star formation properties of their host galaxies, *especially at high-z, at the height of the SFR and quasar activity.*

With the imminent launch of the James Webb Space Telescope, we will answer several fundamental facts remain unknown for high-luminosity AGN, i.e. quasars: What is the main AGN triggering mechanism at the height of quasar activity at redshifts $z = 2 - 3$? What is the direct, observational evidence in individual objects, that links AGN activity to star formation? Can we observe "AGN feedback" in action, in situ for the most luminous sources at their peak activity?

Our team has discovered, and has led the field in the characterization of the "Extremely Red Quasar" population, a subset of quasars which we've now shown have very different properties compared to the general quasar population. These are possibly 'very young' quasars and experiencing their first quasar phase. The Extremely Red Quasars are preferentially found at $z \approx 2.5$ the height of the quasar epoch.

Simply put, we want to know the level of star-formation in these Extremely Red Quasars.

The Extremely Red Quasar Population: By matching the quasar catalogues of the Sloan Digital Sky Survey (SDSS), the Baryon Oscillation Spectroscopic Survey (BOSS) to the Wide-Field Infrared Survey Explorer (WISE), Ross et al. (2015) discovered quasars with extremely red infrared-to-optical colours: $r_{\rm AB} - W4_{\rm Vega} > 14$ mag, i.e., $F_\nu(22\mu{\rm m})/F_\nu(r) \gtrsim 1000$. These objects have infrared luminosities $\sim 10^{47}$ erg s^{-1}. The original motivation here was to look for PAHs that had redshifted in the WISE W4 band for $z \approx$2.5 quasars in order to study and link luminous AGN activity and star formation at the "height of the quasar epoch".

Hamann et al. (2017) then fully and properly refined the selection of the ERQs, changed the definition based on other data and common properties, and indeed found many more objects in this new scheme. The ERQs have a suite of peculiar emission-line properties including large rest equivalent widths (REWs), unusual "wingless" line profiles, large N V/Lyα, N V/C IV, Si IV/C IV and other flux ratios, and very broad and blueshifted [O III] λ5007.

In Hamann et al., our team identified a "core" sample of 97 ERQs with nearly uniform peculiar properties selected via i–$W3 \geq 4.6$ (AB) and REW(C IV) ≥ 100 Å at redshifts 2.0–3.4. A broader search finds 235 more red quasars with similar unusual characteristics. The core ERQs have median luminosity $\langle \log L(\mathrm{ergs/s}) \rangle \sim 47.1$, sky density 0.010 deg^{-2}, surprisingly flat/blue UV spectra given their red UV-to-mid-IR colors, and common outflow signatures including BALs or BAL-like features and large C IV emission-line blueshifts. Their SEDs and line properties are inconsistent with normal quasars behind a dust reddening screen. These "Core ERQs" are a unique obscured quasar population with extreme physical conditions related to powerful outflows across the line-forming regions. Patchy obscuration by small dusty clouds could produce the observed UV extinctions without substantial UV reddening.

In Zakamska et al. (2016) we used XShooter/VLT to measure rest-frame optical spectra of four $z \sim 2.5$ extremely red quasars. We discovered very broad (full width at half max= $2600-5000$ km s^{-1}), strongly blue-shifted (by up to 1500 km s^{-1}) O III $lambda$5007Å emission lines in these objects. In a large sample of type 2 and red quasars, O III kinematics are positively correlated with infrared luminosity, and the four objects in our sample are on the extreme end both in O III kinematics and infrared luminosity. As such, we estimate that at least 3% of the bolometric luminosity in these objects is being converted into the kinetic power of the observed wind. Photo-ionization estimates suggest that the O IIIemission might be extended on a few kpc scales, which would suggest that the extreme outflow is affecting the entire host galaxy of the quasar. These sources may be the signposts of the most extreme form of quasar feedback at the peak epoch of galaxy formation, and may represent an active "blow-out" phase of quasar evolution.

Alexandroff et al. (2017 submitted and in prep.)....

MIR spectroscopy: Fom Veilleux arXiv:0201118v1:: How do galaxies form? How do they evolve? How do supermassive black holes fit in this picture of galaxy formation? Which objects are the main contributors to the overall energy budget of the universe? To properly answer these questions, one will need to differentiate objects powered by nuclear fusion in stars (i.e. normal and starburst galaxies) from objects pow- ered by mass accretion onto supermassive black holes (quasars and AGNs). A wide variety of diagnostic tools have been used in the past for this purpose with different degree of success.

Direct spectroscopy searches for the presence of the broad recombination lines at wavelengths where the effects of dust extinction are reduced. We follow "Veilleux's Commandments":

- Thou shalt use lines which emphasize the differences between H II regions and AGNs; i.e., use high-ionization lines or low-ionization lines produced in the partially ionized zone.

- Thou shalt use strong lines which are easy to measure in typical spectra.
- Thou shalt avoid lines which are badly blended with other emission or absorption line features.
- Thou shalt use lines with small wavelength separation to minimize sensitivity to reddening.
- Thou shalt use line ratios from the same elements or involving hydrogen recombination lines to eliminate or reduce abundance dependence.
- Thou shalt avoid lines from Mg, Si, Ca, Fe depleted onto dust grains.
- Thou shalt avoid lines affected by strong stellar absorption features.
- Thou shalt avoid lines affected by strong atmospheric features.
- Thou shalt use lines at long wavelengths to reduce the effects of dust extinction.

From Padovani et al., arXiv:1707.07134v1 IR spectroscopy, particularly with the InfraRed Spectrograph (IRS; Houck et al. 2004) on board the Spitzer Space Telescope, provided new insights into the physics and classification of AGN. The unambiguous observations of the sil icate feature at 9.7 μm in emission in many known AGN (Hao et al., 2005; Siebenmorgen et al., 2005; Sturm et al., 2005; Buchanan et al., 2006; Shi et al., 2006) came as the long sought confirmation of the unified scheme. At the same time, however, IRS observations indicated that in some cases the source of obscuration resides in the host rather than the torus (e.g. Goulding et al., 2012; Hatziminaoglou et al., 2015). Identification through MIR spectroscopy is very powerful, allowing to detect obscured AGN components even when the MIR is dominated by the host galaxy. Several classification diagrams have been developed to determine the AGN contribution to an observed spectrum based on certain spectral features, such as high ionisation emission lines like Ne V , [Ne II] and O IV, the EW of PAH features and the strength of the silicate feature at 9.7 μm (see, e.g. Spoon et al., 2007; Armus et al., 2007; Veilleux et al., 2009; Hernan-Caballero & Hatziminaoglou, 2011). A number of techniques have also been developed to model the observed MIR spectra and constrain the AGN and starburst contributions (see e.g. Schweitzer et al., 2008; Nardini et al., 2008; Deo et al., 2009; Feltre et al., 2013). Although MIR spectroscopy has had a great impact on our understanding of AGN, the number of objects studied through these techniques is limited when compared to photometric studies, as spectroscopic observations require significantly longer integration times. Ground-based observations are generally limited to the brightest targets due to the effects of the Earth's atmosphere (e.g. Alonso-Herrero et al., 2016), while deeper observations were possible with the IRS during its cryogen-cooled phase. For the most part, such observations were limited to z 1 luminous IR galaxies (LIRGs), ultraluminous IR galaxies (ULIRGs), and quasars (Hernan-Caballero & Hatziminaoglou, 2011, and references therein) although a number of higher redshift ULIRGs were also studied by IRS (see e.g. Kirkpatrick et al., 2012). The impact of these techniques will be greatly expanded by the upcoming JWST (Gardner et al. 2006) (and Space Infrared Telescope for Cosmology and Astrophysics, SPICA; Nakagawa et al. 2015), that will probe significantly fainter targets and will allow us to select new, currently inaccessible, sets of objects, as discussed next.

Polycyclic Aromatic Hydrocarbons: Polycyclic Aromatic Hydrocarbons (PAHs) are abundant, ubiquitous, and a dominant force in the interstellar medium of galaxies (see e.g., Tielens, 2008, ARAA, 46, 289 for a review). Aromatic features are already a significant component of dusty galaxy spectra as early as $z \approx 2$ (Yan et al., 2005, ApJ, 628, 604). and the infrared (IR) emission features at 3.3, 6.2, 7.7, 8.6, and 11.3 μm are generally attributed to IR fluorescence from (mainly) far-ultraviolet (FUV) pumped large polycyclic aromatic hydrocarbon (PAH) molecules. As such, these features trace the FUV stellar flux and are thus a measure of star formation (Peeters et al, 2004, ApJ, 613, 986). Given the redshift of our ERQs and the MIRI wavelength coverage we will coverage $1.36 \leq \lambda_{\rm emitted} \leq 8.6\mu$m.

Relation to Spitzer IRS: Major Achievement of Spitzer was IRS.
$R \sim 600$, now $R \sim 2000s$, which allows *chemistry.*
Spitzer IRS died before WISE; therefore now WISE W4 objects were observed by the IRS.
i.e. no $z \sim 2.5$ ERQs w/ feedback in action were observed.

MIRI Imaging: Imaging of the ERQs will tell us what environments they live in (currently totally unknown).
Just look at the ERQs: flux from central source $\Rightarrow$ AGN; flux from extended $\Rightarrow$ SF; Big puzzle since Spitzer (e.g. and cf. the submm population).

Next Steps:

Technical Description

Describe the targets and observational modes to be used. Quantitative estimates must be provided of the accuracy required to achieve key science goals. Proposers must demonstrate that all observations can execute in the first 5 months of Cycle 1 (planned to be from April to August 2019), and that a substantive subset of the observations are accessible in the first 3 months. This description should also include the following::

a Plan for Alternative Targets: As described in JWST DD ERS Special Observational Policies, proposers should qualitatively describe the availability of alternate targets and the process used to identify those targets should the start of science observations be delayed. Robust ERS programs involve science investigations that can be performed with a variety of different targets and observations.

b Special Observational Requirements (if any): Justify any special scheduling requirements, e.g., time-critical observations.

c Justification of Coordinated Parallels (if any): Proposals that include coordinated parallel observations should provide a scientific justification for and description of the parallel observations. It should be clearly indicated whether the parallel observations are essential to the interpretation of the primary observations or the science program as a whole, or whether they address partly or completely unrelated issues. The parallel observations are subject to scientific review, and can be rejected even if the primary observations are approved.

d Justification of Duplications (if any): as detailed in the JWST DD ERS Proposal Policies and the JWST Duplicate Observations Policy, observations taken as part of the DD ERS program cannot duplicate those specified for the GTO Cycle 1 Reserved Observation Catalog (planned for release on June 15, 2017). Any duplicate observations must be explicitly justified.

Object Name (SDSS)	J0834+0159	J1232+0912	J2215-0056	J2323-0100
Object R.A.	08:34:48.48	12:32:41.73	22:15:24.00	23:23:26.17
object declination	+01:59:21.1	+09:12:09.3	−00:56:43.8	−01:00:33.1
r-band AB magnitude	21.20±0.05	21.11± 0.05	22.27±0.12	21.62± 0.08
Redshift $z_{\rm in}$	2.591	2.381	2.509	2.356
CIV FWHM km s^{-1}	2863±65	4787±52	4280±112	3989±62
O III FWHM erg s^{-1}	2811	4971	3057	2625
Spectro-polarimertry	×	$\surd$	$\surd$	×
VLA data	?	?	?	?
ALMA Band 6	tbc	$\surd$	tbc	$\surd$
JWST target visibility (Start)	2019-04-01	2019-05-08	2019-05-22	2019-06-07
JWST target visibility (End)	2019-05-07	2019-07-01	2019-07-15	2019-07-29

■ Plan for Alternative Targets

■ Special Requirements

■ Justify Coordinated Parallel Observations

■ Justify Duplications

Data Processing & Analysis Plan

1 `mrs_analyzer`

`mrs_analyzer` is a Python module for analyzing MRS data; `mrsfringe` is a Python module for mitigating MRS fringing issues;

And will integrate with... `https://github.com/STScI-JWST`
see e.g. `https://github.com/STScI-JWST/jwst/blob/master/jwst/mrs_imatch/mrs_imatch_step.py`

2 The NASA Ames PAH IR Spectroscopic Database

We will link to the NASA Ames PAH IR Spectroscopic Database::
http://www.astrochem.org/pahdb/
Bauschlicher et al, 2010, ApJS, 189, 341; Boersma et al, 2014, ApJS, 211, 8; Mattioda et al., ApJS, in prep.

3 PandExo: An Exoplanet ETC

`https://natashabatalha.github.io/PandExo/`

4 The SMART Data Analysis Package for the Infrared Spectrograph1 on the Spitzer Space Telescope

The SMART Data Analysis Package for the Infrared Spectrograph on the Spitzer Space Telescope from S. J. U. Higdon,3 D. Devost,3 J. L. Higdon,3 B. R. Brandl,4 J. R. Houck,3 P. Hall,3 D. Barry,3 V. Charmandaris,3,5 J. D. T. Smith,6 G. C. Sloan,3 and J. Green7 Publications of the Astronomical Society of the Pacific, 116:975984, 2004 October.

5 Delivery Schedule for Science-Enabling Products.

Here we give the delivery schedule for science-enabling products. Proposals must present a delivery schedule for science-enabling products. A description of STScI pipeline data products, processing and analysis software, and their anticipated availability, will be provided by the May 2017 release of the final version of this Call for Proposals. Proposers may consider multiple deliveries, with more advanced products provided over longer timescales. Proposals may include the collection, processing and analysis of ancillary data as part of an integrated DD ERS proposal.

6 Co-Investigators and Delivery of Science-Enabling Products.

Co-Investigators, together with the PI (and any Co-PIs) comprise a core team with the responsibility of developing and delivering science-enabling products as described in the proposal, as well as carrying out selected key aspects of the science investigations. A Co-I must have a well-defined, and generally sustained, continuing role in team activities, serve under the direction of the PI, or co-PI(s). Co-investigators may or may not receiving funding, pending eligibility, through the DD ERS program.

6.1 Dr. Nicholas Ross

P.I. Dr. Nic Ross is a deep believer in delivering science-enabling products, including datasets, catalogs, analysis codes, plots, algorithms and where possible computational resources to the wide astronomical community. As such, the call for delivering science-enabling products by the release of the Cycle 2 Call for Proposals (September 2019) is fully inline with his scientific practice.

Ross has being developing and buidling up his GitHub Repositories over the last year or so, `github.com/d80b2t` and indeed now does all his analysis and paper writing on GitHub.

Ross will devote a considerable amount of his personal research time (and due to his STFC ERF has 100% FTE for research) to leading the developement and timely prodcution of the ERS ERQ science-enabling products.

6.2 Dr. David Rosario

. Co-PI Dr. David Rosario is awesome and loves also writing code.

6.3 Prof. David Alexander

Prof. Alexander is an expert in high-z obsured AGN. He will use his considerable *Spitzer IRS* expereince to help test our MIRI MRS data-analysis toolkit.

6.4 Dr. Rachael Alexandroff

Dr. Alexandroff is an leading expert on the ERQ population. She will bring to bear her now considerable and recent data analysis (long-slit optical, polarimerty, radio) data analysis experience to build our MIRI MRS data-analysis toolkit.

6.5 Dr. Richard Bielby

6.6 Prof. Beth Biller

6.7 Prof. Niel Brandt

6.8 Dr. Rob Crain

6.9 Prof. Xiaohui Fan

6.10 Prof. Fred Hamann

6.11 Prof. Dale Kocevski

6.12 Prof. Linhua Jiang

6.13 Dr. Stephanie LaMassa

6.14 Dr. Chelsea MacLeod

6.15 Dr. Ian McGreer

6.16 Prof. Brice Menard

6.17 Dr. James Mullaney

6.18 Prof. Adam Myers

6.19 Dr. Jessie Runnoe

6.20 Prof. Don Schneider

6.21 Prof. Tom Shanks

6.22 Dr. John Stott

6.23 Prof. Michael Strauss

6.24 Dr. Renske Smit

6.25 Prof. Martin Ward

6.26 Prof. Gillian Wright

6.27 Prof. Nadia Zakamsaka