

Abstract Type	Research Contributed Presentations
Presentation Type	Oral
First Category	Invited
Student Status	Not a student
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Newsworthy	No

Experimental and theoretical needs for the JWST Early Release Science Program on radiative feedback from massive stars (PDRs4ALL): III. A quantum chemistry perspective

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Massive stars disrupt their natal molecular cloud material by dissociating molecules, ionizing atoms and molecules, and heating the gas and dust. These processes drive the evolution of interstellar matter in our Galaxy and throughout the Universe from the era of vigorous star formation at $z=1-3$ to the present day. Much of this interaction occurs in Photo-Dissociation Regions (PDRs) where far-ultraviolet photons of these stars create a largely neutral, but warm region of gas and dust. PDR emission dominates the IR spectra of star-forming galaxies and provides a unique tool to study the physical and chemical processes that are relevant for inter- and circumstellar media including diffuse clouds, molecular cloud and protoplanetary disk surfaces, and starburst galaxies.

The ERS program ID1288 is dedicated to provide template data as well as data processing and analysis tools for PDRs. To this end, it will observe the Orion Bar, the proto-typical PDR situated in the nearby Orion Nebula, using NIRSpec IFU, MIRI IFU, and NIRCAM and MIRI imaging. These observations will, for the first time, spatially resolve and perform a tomography of the PDR, revealing the individual IR spectral signatures from the key zones and sub-regions within the ionized gas, the PDR, and the molecular cloud.

Quantum chemistry can be used to determine molecular data such as ionization potentials, chemical reaction rates, electronic spectra, dissociation energies, channels, and branching ratios, etc. These are often used in synergy with experiment to take advantage of the strengths of each approach. An area of active research is modeling the infrared (IR) emission spectra produced by PAH molecules, including the effects of anharmonicity. This will be important in the interpretation of JWST data which will yield higher-resolution spectral data compared to Spitzer or ISO. Quantum chemistry methods can compute accurate anharmonic IR absorption spectra of PAH molecules up to about 25 C atoms, and the results have been benchmarked against high-resolution experimental spectra. These feed into a quantum Monte Carlo (QMC) approach to generate temperature-dependent anharmonic IR emission spectra and then used to generate fully anharmonic cascade emission IR spectra of PAH molecules -- the very type of spectra that JWST will observe. Work continues to extend these methods to larger PAH molecules. We will discuss the current state of this work, as well as the current state of quantum chemistry methodology that can be used for determining some of the other physical parameters needed in the interpretation of JWST observations.

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