EAPS Planetary lunch Colloquium Series (PICS)

Dr. Clara Sousa-Silva
Postdoctoral Associate
Massachusetts Institute of Technology

Tuesday, October 31st
12:30pm
54-517

Simulations of molecular spectra for detection of biosignature gases and other volatiles

The ability to identify molecules within spectra is of importance for a variety of scientific and industrial uses. A compelling modern focus is the spectroscopic detection of biosignature gases on exoplanets. A comprehensive analysis of any given observational spectra requires information about the spectrum of each of its molecular components. However, knowledge of molecular spectra currently only exists for a few hundred molecules and, other than a handful of exceptions (e.g. H_2O, NH_3), most of their spectra are incomplete.
Given the relatively low level of accuracy that observations often require, there is value in creating approximate simulated spectra of molecules, particularly for those about which we know very little or nothing at all. ATMOS (Approximate Theoretical MOlecular Spectra) provides approximate spectra for thousands of molecules in a computationally expedient manner, using a combination of experimental measurements, organic chemistry, and quantum mechanics. ATMOS 1.0, presented here, can identify volatile molecules with significant spectral features in any given wavelength window within the infrared region and provide spectral information about the main features of most molecules.

For more information, contact John Biersteker (jo22395@mit.edu)

EAPS
Earth, Atmospheric and Planetary Sciences