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First-Principles Molecular Spectra of Air MARK ZAMMIT, JULIE JUNG, JEFFERY LEIDING, Los Alamos National Laboratory — Comprehensive and highly accurate rovibronic spectral measurements of air molecules are critical to the modeling of low-temperature plasmas and air in extreme conditions. However, with the lack of experimental data, first-principles approaches are key to generating complete molecular line lists. Here, we will discuss the methodology employed for the accurate calculation of molecular rovibronic states, and present emission and equation of state results for NO and OH, which form in significant abundance in air under extreme conditions.

Mark Zammit
Los Alamos National Laboratory

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