THEORETICAL TOOLS FOR MOLECULAR DISCOVERY IN THE LABORATORY AND SPACE

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First-principles calculations of the rovibronic structure, spectra, and properties of polyatomic molecules often resist a "one-size-fits-all" approach, reflected by the wide variety of theoretical tools available for these problems. A common trait shared by many of these methods is the need for efficient and accurate derivatives (occasionally to high order) of multivariate quantities with complex functional forms including potential energy surfaces, curvilinear coordinate systems, frame embeddings, and basis functions. This talk will outline the use of automatic differentiation techniques to simplify the design and implementation of versatile rovibrational methods with a particular focus on generating predictions and insights for high-resolution microwave and optical spectroscopy of small molecules. The application of these and other tools will be highlighted with several recent results from our group, including the laboratory and astronomical discovery of new metal-bearing dicarbides, the structure and electronic properties of laser-coolable polyatomic molecules, and the hyperfine-resolved microwave spectroscopy of reactive, open-shell hydrocarbons.