QUANTUM SCATTERING CALCULATIONS FOR ACCURATE MODELING OF COLLISION-PERTURBED MOLECULAR SPECTRA

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Reliable interpretation of molecular spectra requires taking into account subtle collisional effects that extend beyond the Voigt profile. Such effects include spatial confinement of molecules due to frequent velocity-changing collisions, which gives rise to the Dicke narrowing phenomenon,[1] and the speed dependence of collisional broadening and shift.[2]

I will present a theoretical description of the shapes of molecular resonances, based on *ab initio* potential energy surfaces, quantum scattering calculations, and an advanced statistical model of collisional perturbation of the optical coherence. This approach has been successfully validated on cavity-enhanced spectra of H_2 perturbed by collisions with He atoms[3] and H_2-perturbed D_2 lines. I will discuss the challenges in performing quantum scattering calculations in diatom-diatom systems and the computational tools developed in our group. I will present the application of the theoretical approach in accurate spectroscopy of hydrogen for fundamental studies[4] and the importance of beyond-Voigt line-shape effects in the context of astrophysical spectral analysis and terrestrial atmospheric studies. In particular, I will highlight our results for resonances in CO,[5,6] O_2[7] and HCl, perturbed by collisions with the most abundant species of the Earth's atmosphere: N_2 and O_2.

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