

AB INITIO LINE-SHAPE CALCULATIONS

¹Piotr Wcisło, ²Franck Thibault, ¹Hubert Cybulski, ¹Roman Ciuryło



¹Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudziądzka 5, 87-100 Toruń, Poland ²Institut de Physique de Rennes, UMR CNRS 6251, Université de Rennes 1, Campus de Beaulieu, Bât.11B, F-35042 Rennes, France

What?

We performed ab initio calculations of the shapes of self-, Ar- and He-perturbed H₂ and D₂ rovibrational lines [1, 2].

- We performed highly accurate ab initio calculations of the three dimensional H₂-Ar potential energy surface (PES).
- We calculated generalized cross sections for line broadening and shifting by solving the close-coupling (CC) equations.
- We used a hard-sphere approximation of the H_2 -X potentials to describe velocity-changing collisions.
- We simulated the shapes of H₂/D₂ lines by solving the transport/relaxation equation for optical coherences [3,4].



Fundamental discrepancies between thermally averaged collisional broadening obtained experimentally [5,6] and from ab initio close-coupling (CC) calculations were reported [7-9].

- To understand the role of the velocity-changing collisions on the anomalous inhomogeneity in H₂/D₂ line broadening.
- The *ab initio* model of molecular line shape is essential to eliminate systematic errors in optical metrology based on molecular spectroscopy [10].
- Validation of the ab inition quantum-chemical calculations of PESs [11].
- The shapes of H₂ spectra are starting to be important for astrophysical studies, especially for the studies of the atmospheres of giant planets [12].



COMPARISON WITH EXPERIMENTAL DATA



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v (10⁻³ cm⁻¹

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