

**UV and IR absorption spectrum of nitrogen dioxide and water dimer:
assessing the accuracy of electronic structure calculations and experiments.**

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Abstract:

NO₂ and water are important gases in the atmosphere. NO₂ which is also a trace gas is produced naturally and industrially. NO₂ in the atmosphere absorbs sunlight and contributes in regulating the chemistry of the troposphere and the concentration of ozone. Industrially, it is an intermediate in the synthesis of nitric acid which are used for the production of fertilizers, it contributes to the manufacturing of explosives or even acts as an oxidizer in rocket fuel. Water, often called the ‘molecule of life’, is on its own one of the most studied molecule to date, owing to its importance. In our talk we will present new calculations and results on the temperature dependent UV absorption spectrum of NO₂ and the infrared spectrum of H₂O-H₂O (the simplest water cluster) in the light of recent¹ and past experiments. In particular, a quantum dynamics description based on the MultiConfiguration Time Dependent Hartree (MCTDH)² approach will be used to study the nuclear motion and predict the various observables. The results of accurate numerical calculations not only provide some insights into the quality of electronic structure calculations and experimental measurements but also suggest areas for improvements in those characterization.

Key-words: Atmosphere, water, nitrogen dioxide, quantum dynamics, MCTDH.

1. Bingbing Zhang, J. Phys. Chem. Lett. 11, 851-855 (2020).
2. M.H. Beck et al., Phys. Rep. 324, 1 (2000).