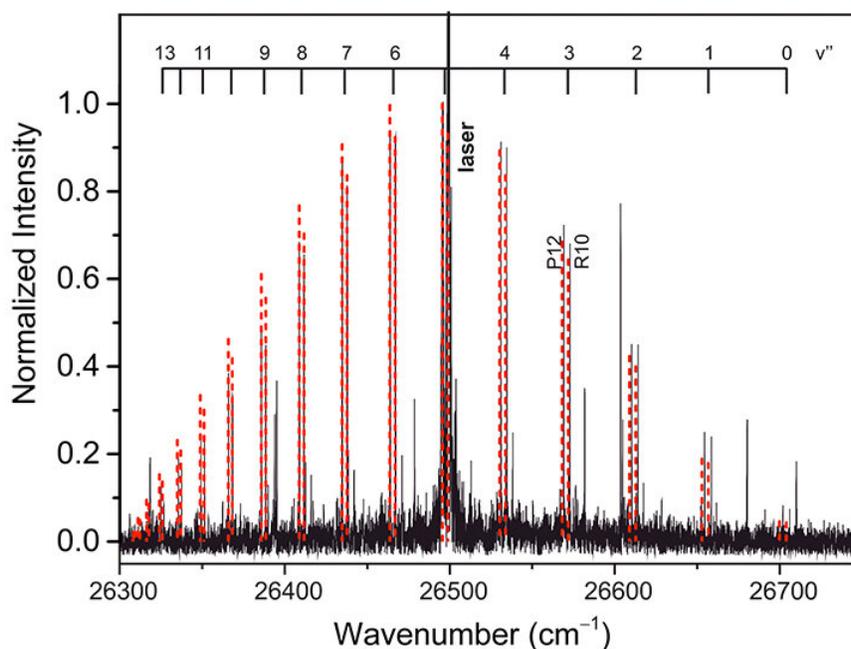


Scientists solve half-century-old magnesium dimer mystery

May 22 2020, by Val Osowski



This graph shows the team's highly accurate ab initio calculations in red, dotted lines relative to the experimental LIF spectrum of Mg₂, marked in black. Credit: Piecuch Lab

Magnesium dimer (Mg₂) is a fragile molecule consisting of two weakly interacting atoms held together by the laws of quantum mechanics. It has recently emerged as a potential probe for understanding fundamental

phenomena at the intersection of chemistry and ultracold physics, but its use has been thwarted by a half-century-old enigma—five high-lying vibrational states that hold the key to understanding how the magnesium atoms interact but have eluded detection for 50 years.

The lowest fourteen Mg_2 vibrational states were discovered in the 1970s, but both early and recent experiments should have observed a total of nineteen states. Like a quantum cold case, experimental efforts to find the last five failed, and Mg_2 was almost forgotten. Until now.

Piotr Piecuch, Michigan State University Distinguished Professor and MSU Foundation Professor of chemistry, along with College of Natural Science Department of Chemistry graduate students Stephen H. Yuwono and Ilias Magoulas, developed new, computationally derived evidence that not only made a [quantum leap](#) in first-principles quantum chemistry, but finally solved the 50-year-old Mg_2 mystery.

Their findings were recently published in the journal *Science Advances*.

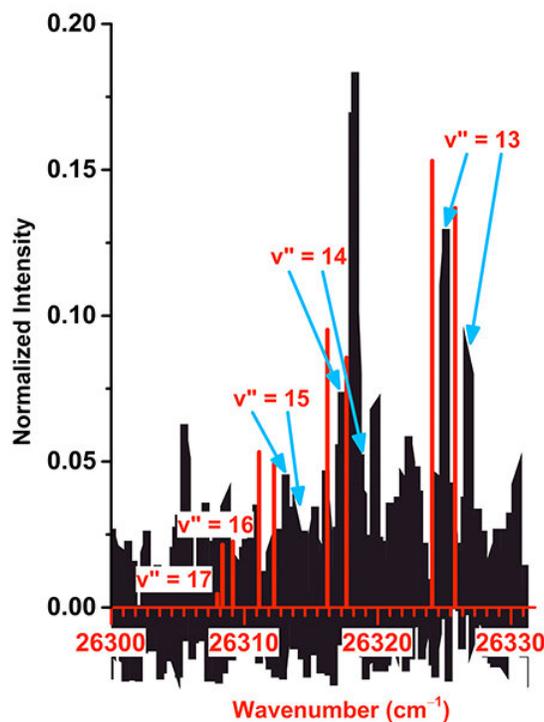
"Our thorough investigation of the magnesium dimer unambiguously confirms the existence of 19 vibrational levels," said Piecuch, whose research group has been active in quantum chemistry and physics for more than 20 years. "By accurately computing the ground- and excited-state potential energy curves, the transition dipole moment function between them and the rovibrational states, we not only reproduced the latest laser-induced fluorescence (LIF) spectra, but we also provided guidance for the future experimental detection of the previously unresolved levels."

So why were Piecuch and his team able to succeed where others had failed for so many years?

The persistence of Yuwono and Magoulas certainly revived interest in

the Mg_2 case, but the answer lies in the team's brilliant demonstration of the predictive power of modern electronic structure methodologies, which came to the rescue when experiments encountered unsurmountable difficulties.

"The presence of collisional lines originating from one molecule hitting another and the background noise muddled the experimentally observed LIF spectra," Piecuch explained. "To make matters worse, the elusive high-lying vibrational states of Mg_2 that baffled scientists for decades dissipate into thin air when the molecule starts rotating."



The missing, high-lying vibrational states of Mg_2 are clearly visible here as computationally derived red lines. Experiments were unable to detect these vibrations—a decades-old enigma the MSU team finally solved. Credit: Piecuch Lab

Instead of running costly experiments, Piecuch and his team developed efficient computational strategies that simulated those experiments, and they did it better than anyone had before.

Like the quantized vibrational states of Mg_2 , in-between approximations were not acceptable. They solved the electronic and nuclear Schrödinger equations, tenets of quantum physics that describe molecular motions, with almost complete accuracy.

"The majority of calculations in our field do not require the high accuracy levels we had to reach in our study and often resort to less expensive computational models, but we provided compelling evidence that this would not work here," Piecuch said. "We had to consider every conceivable physical effect and understand the consequences of neglecting even the tiniest details when solving the quantum mechanical equations."

Their calculations reproduced the experimentally derived vibrational and rotational motions of Mg_2 and the observed LIF spectra with remarkable precision—on the order of 1 cm^{-1} , to be exact. This provided the researchers with confidence that their predictions regarding the magnesium dimer, including the existence of the elusive high-lying vibrational states, were firm.

Yuwono and Magoulas were clearly excited about the groundbreaking project, but emphasized they had initial doubts whether the team would be successful.

"In the beginning, we were not even sure if we could pull this investigation off, especially considering the number of electrons in the magnesium dimer and the extreme accuracies required by our state-of-the-art computations," said Magoulas, who has worked in Piecuch's research group for more than four years and teaches senior level

quantum chemistry courses at MSU.

"The computational resources we had to throw at the project and the amount of data we had to process were immense—much larger than all of my previous computations combined," added Yuwono, who also teaches physical chemistry courses at MSU and has worked in Piecuch's research group since 2017.

The case of the high-lying [vibrational states](#) of Mg₂ that evaded scientists for half a century is finally closed, but the details of the computations that cracked it are completely open and accessible on the Science Advances website. Yuwono, Magoulas, and Piecuch hope that their computations will inspire new experimental studies.

"Quantum mechanics is a beautiful mathematical theory with a potential of explaining the intimate details of molecular and other microscopic phenomena," Piecuch said. "We used the Mg₂ mystery as an opportunity to demonstrate that the predictive power of modern computational methodologies based on first-principles quantum mechanics is no longer limited to small, few-electron species."

More information: Stephen H. Yuwono et al, Quantum computation solves a half-century-old enigma: Elusive vibrational states of magnesium dimer found, *Science Advances* (2020). [DOI: 10.1126/sciadv.aay4058](https://doi.org/10.1126/sciadv.aay4058)

Provided by Michigan State University

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