FINAL REPORT

The principal results achieved during my last NKFIH-OTKA grant, K119658, entitled "Molecules in Motion", have been made accessible in 69 scientific publications[102-170] (the first 101 publications listed were supported by my previous three OTKA grants; I'm listing them here as they provide background material to many of the recent achievements). The D1 journals we chose to publish our results in include *Nat. Commun.*, *Chem. Comm.*, *WIRES Comput. Mol. Sci.*, *Astrophys. J. Suppl.*, *JCTC*, and *JPCL*, while the majority of the results have been published in Q1 journals including *J. Chem. Phys.*, *Phys. Chem. Chem. Phys.*, *J. Quant. Spectrosc. Rad. Transf.*, and *J. Phys. Chem. Ref. Data*. The cumulative impact factor of these papers is above 250. As seen in Fig. 1, Web of Science lists 53 publications with support received through grant no. K119658, while Fig. 2 shows that these publications received 566 citations in total (as of October 6, 2021).

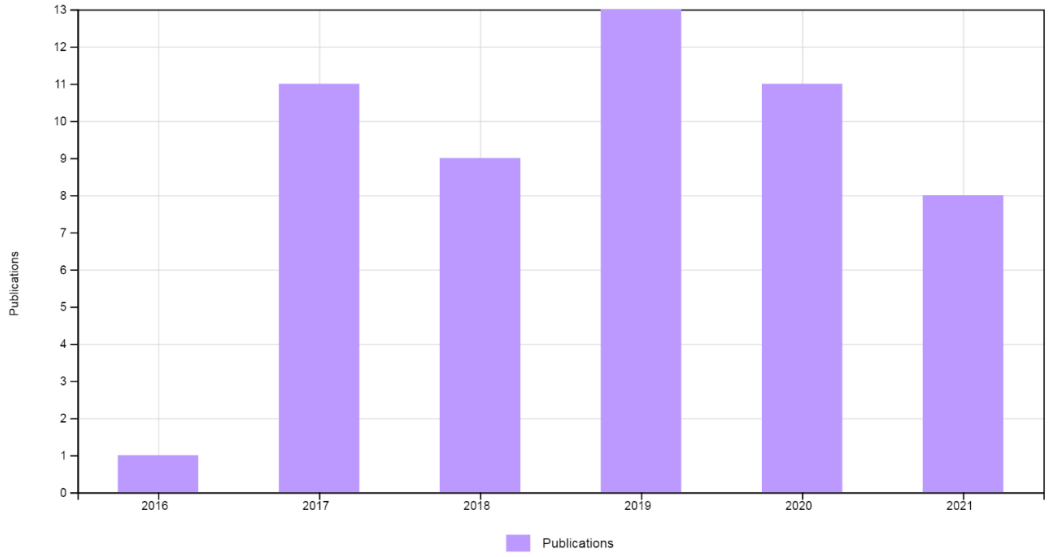


Fig. 1. The yearly distribution of publications with the acknowledgement of grant K119658, as provided by the Web of Science (note that this is an incomplete list, containing 53 out of the 69 supported publications)

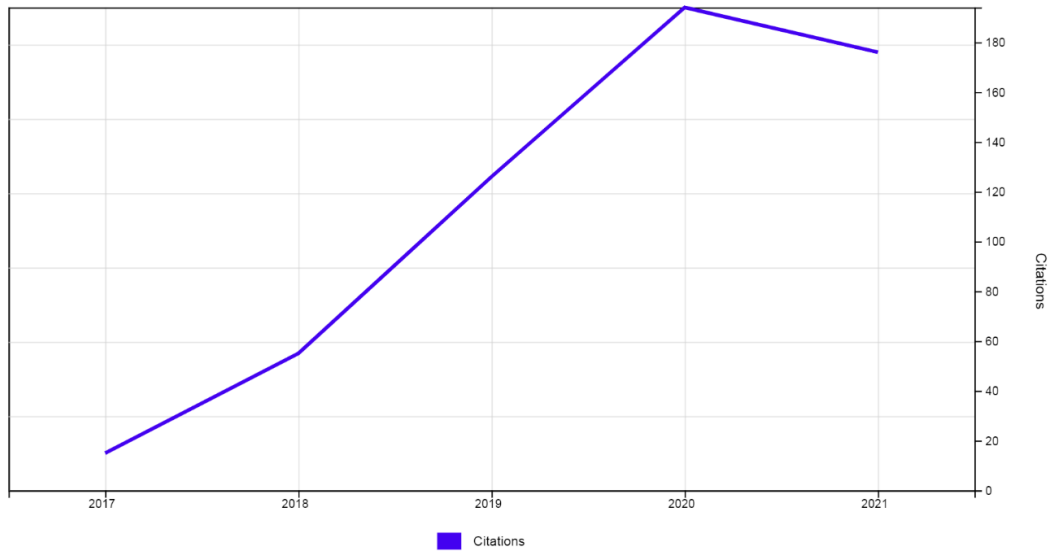
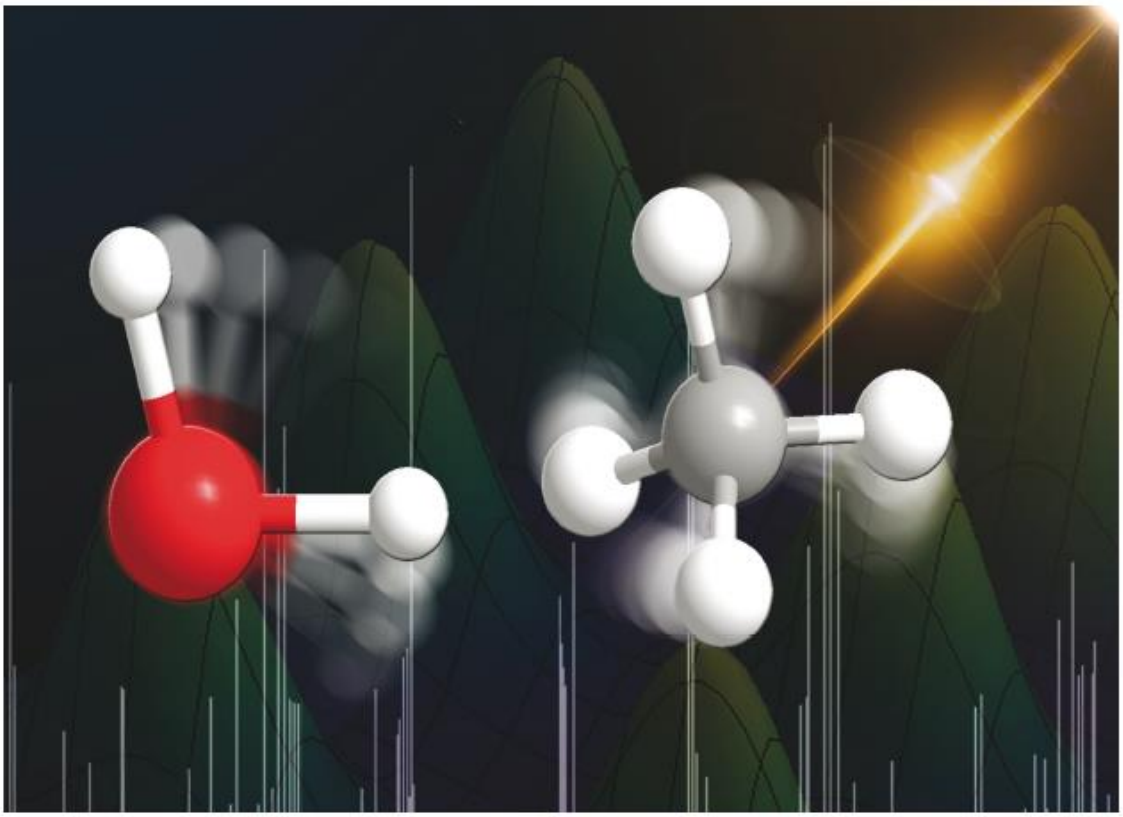


Fig. 2. The yearly distribution of citations of papers acknowledging grant K119658, as maintained by the Web of Science (WoS, note that this is an incomplete list, as the WoS search identified only 53 out of the 69 publications with grant support)



Showcasing research from the Laboratory of Molecular Structure and Dynamics, Institute of Chemistry, Eötvös Loránd University, Budapest, Hungary

Title: Rovibrational transitions of the methane–water dimer from intermolecular quantum dynamical computations

Quantum dynamical computations of the weakly bound, highly fluxional methane–water dimer explain high-resolution far-infrared spectroscopic measurements and validate the intermolecular model potentials of this prototype of the water hydrocarbon interactions.

As featured in:

See Edit Mátyus *et al.*, *Phys. Chem. Chem. Phys.*, 2016, **18**, 22816.

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Fig. 3. Our 2016 paper "Rovibrational transitions of the methane-water dimer from intermolecular quantum dynamical computations" on the cover of *Phys. Chem. Chem. Phys.*,[107] a journal of the Royal Society of Chemistry.

Most of the 69 papers published were well received by the scientific community, as can be judged by the number of citations they attracted (see Fig. 2). I'm especially pleased that the H-index of the 53 NKFIH-supported publications in WoS is as high as 14, even though the first papers were published only in 2016, that is only five years ago.

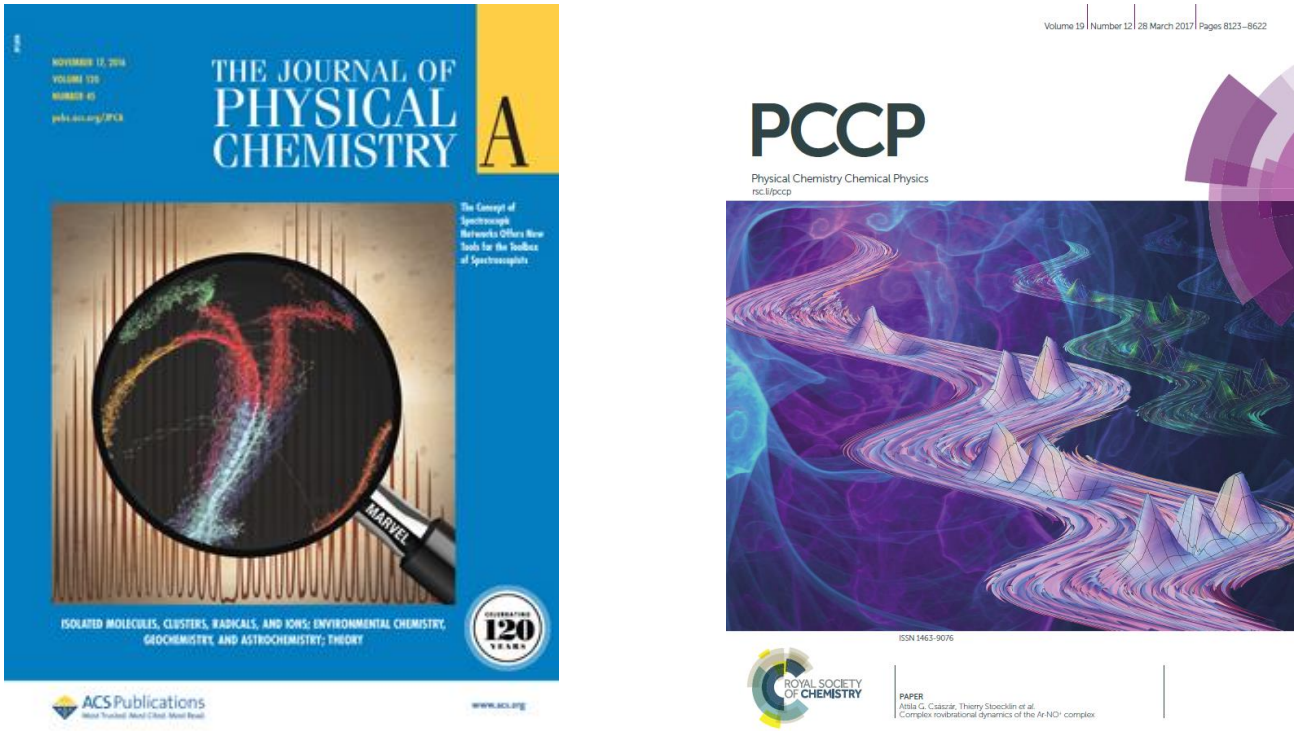

Fig. 4. (a) Our 2016 paper "Small Molecules – Big Data" on the front cover of *J. Phys. Chem. A*,[108] a journal of the American Chemical Society and (b) our 2017 paper on the front cover of *Phys. Chem. Chem. Phys.*,[111] a journal of the Royal Society of Chemistry.

The results obtained could not have been achieved just by myself. Thus, hereby I'd like to acknowledge the help I received from the following persons who have been supported by the grant for a shorter or longer period of time: Dr. Csaba Fábri (2016-2017), Dr. Tibor Furtenbacher (2017-2018, 2020-2021), Ms. Irén Simkó (2017-2019), and Dr. Péter Árendás (2020-2021). Note also that a number of my papers[102-170] have co-authors not only from Hungary but also from abroad. In the present era of theoretical chemistry, experiment and theory provide resources that clearly complement each other and both are needed to make scientific progress. In several joint publications the non-Hungarian co-authors were involved to do the experiments required (see the joint publications with the groups of B. Drouin, S. Schlemmer, W. Ubachs, and X. Zeng). In some other cases, the co-authors are long-time collaborators in the field of molecular physics, such as Prof. Jonathan Tennyson and his group from UCL and Prof. Laura McKemmish (Australia). It is important to point out that several of our publications ended up on the cover of the journals in which they were published in[107,108,111,151,156,165] (see Figs. 3-6 for some of these covers representing a number of research topics supported by the NKFIH-OTKA grant).

Methodological achievements

During the course of the K119658 project, I introduced a number of new theoretical, in particular quantum-chemical and numerical techniques to quantum dynamics (QD), high-resolution spectroscopy, and beyond.[116,117,126,127,132,138,141,147,151,157] Some of these achievements extended previous approaches I developed[9,36,50,51,55,84,91] with the support of previous OTKA grants. These developments serve, in particular, the "fourth age of quantum chemistry".[61] The related achievements allow the characterization of a large number of stationary rovibrational states of polyatomic systems, which in turn allow the first-principles computation of spectra from the microwave to the ultraviolet region and to do QD. Some of the quantum-chemical methods developed[116,141,151,157] allow the computation not only of rovibrational bound but also of so-called resonance (unbound) states,[151] often measurable experimentally. Resonance states are highly important for chemical reactions in the gas phase.

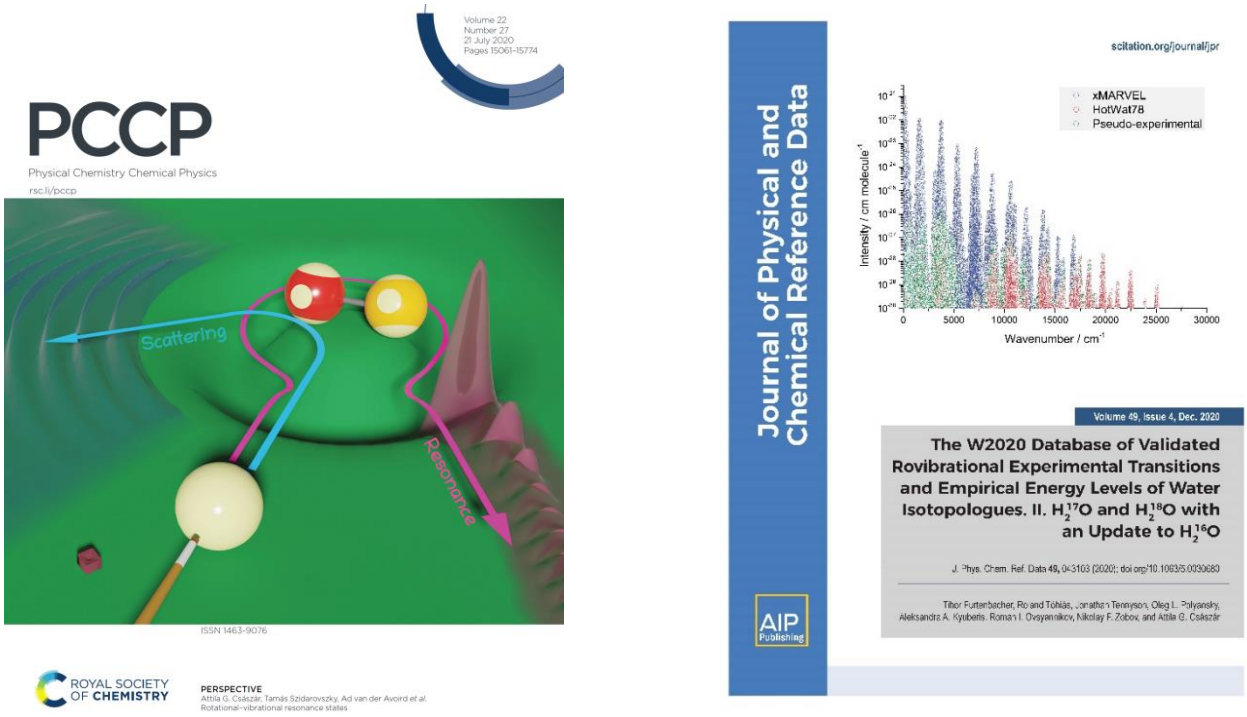

Fig. 5. (a) Our 2020 review-like paper "Rotational-Vibrational Resonance States" on the front cover of *Phys. Chem. Chem. Phys.*,[151] a journal of the Royal Society of Chemistry and (b) our MARVEL-based paper[156] on the front cover of *J. Phys. Chem. Ref. Data*, a journal of the American Institute of Physics.

The methodological developments include techniques whereby elements of graph (network) theory have been utilized, facilitating studies of high-resolution and ultraprecise molecular spectroscopy.[120,134,148,150,155] Interpretation and utilization of data produced by high-resolution and ultraprecise experimental techniques have been helped by advances in our MARVEL (Measured Active Rotational-Vibrational Energy Levels) protocol,[30,70] which has now been established as the best procedure to treat the openly available experimental data of high-resolution molecular spectroscopy.

Quasistructural molecular systems, a term I introduced into the literature,[146] form a new class of superfluxional, shape-changing molecules. They challenge our definition of molecular shape, molecular motion, and how we envision rotations and vibrations of quantum systems.[146,157] The methodological developments, including symmetry considerations[117] and the introduction of quantum graphs to molecular spectroscopy,[128,164] necessary for the detailed understanding of the dynamical behavior of quasistructural molecules form important elements of the successes of the past five years. Our unusual modeling efforts, like quantum graphs[128,164] and the rovibrational Aharonov-Bohm effect,[168] should prove useful in the understanding of complex rovibrational phenomena and extending the models chemists use for a qualitative understanding of experimental data.

We made significant progress in the use of network theory to spectroscopy, all built around the concept of spectroscopic networks (SN)[30,31] introduced by us. These developments include, for example, a better understanding of cycles[108] and cycle bases.[120] One of our recent articles[155] also relies heavily on graph theory: the central mathematical concept of this paper is the two-edge-connectivity of a graph. The interdisciplinarity of this area of research is underlined by a PhD degree in mathematics and computer science, earned in 2019 by a former PhD student, Dr. Péter Árendás. We plan to further explore the opportunities where applied mathematics can help solving notable problems of molecular spectroscopy.

We proved,[149] using network theory, that the age-old effective-Hamiltonian approach to model experimental spectra fails if the transitions employed during the fitting form components. We showed, on the example of $^{14}NH_3$,[149] that the error introduced for the rovibrational energies can be huge even when the transitions are fitted perfectly well.

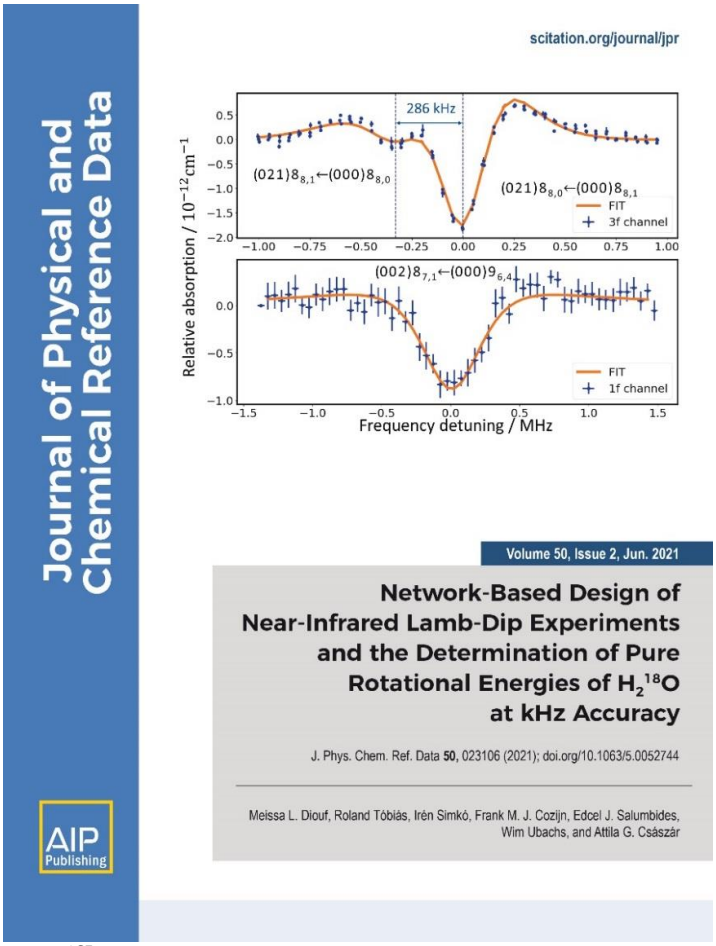

Fig. 6. Our SNAPS-based study[165] from 2021 on the front cover of *J. Phys. Chem. Ref. Data*, a journal of the American Institute of Physics.

In 2020, we have developed the first version of the SNAPS (Spectroscopic Network Assisted Precision Spectroscopy) approach,[148] facilitating the selection of the best lines to measure by optical, precision-spectroscopy (Doppler-free, saturation) experiments, whereby the measurements go line after line, making the experimental effort expensive and time-consumimng. SNAPS selects lines feasible for measurement and with the highest utility. The SNAPS approach has been employed for $H_2{}^{16}O$[148] and $H_2{}^{18}O$[165] *via* the Doppler-free saturation-spectroscopy NICE-OHMS (Noise-Immune Cavity-Enhanced Optical Heterodyne Molecular Spectroscopy) technique (see Fig. 6). SNAPS involves four major phases (see Fig. 9 of Ref. 148): [I] *preparation phase*, whereby the SNAPS input containing information about the accurate transitions governing the selection procedure is created; [II] *selection phase*, where a set of feasible target lines, governed principally by experimental constraints, is generated; [III] *measurement phase*, where, based on a list of target lines, transitions are detected *via* precision spectroscopy; and [IV] *evaluation phase*, where the paths and cycles determined are assessed, improving the input to phase I.

We developed a technique,[133,138] based on the computation of reduced density matrices, for the semi-automatic assignation of vibrational states of arbitrary polyatomic molecules. This is an important aspect of variational nuclear-motion computations to provide a simple physical meaning to the huge number of numerical results.

For he first time after about 80 years, we were able to show numerically the effect of the neglect of the coupling between vibrations and rotations of molecules within different models. We were also able to show, unexpectedly, that there are better embedding schemes than the traditional Eckart embedding.[147,159] Further studies are planned to fully exploit the results obtained.

We published several new and interesting theoretical results[127,130] in the field of light-dressed spectroscopy, writing also a review on the topic.[152] Wave functions resulting from the solution of the nuclear Schrödinger equation, a specialty of our group, are vital in this relatively new field of high-resolution molecular spectroscopy.

Controlling the tunneling behavior of molecules is a highly promising research avenue. In relation to our QD studies providing new theoretical tools, we developed the necessary theoretical and the computational framework on how to achieve tunneling control.[132] We showed quite convincingly, on the example of isotopologues of the ammonia molecule, that both enhancement and inhibition of tunneling and stereomutation dynamics are feasible. This study complemented our earlier investigation of tunneling in ammonia.[100]

Applications

We made significant progress to understand the exceedingly complex dynamics of the quasistructural molecule CH_5^+.[117,128] This molecule, one of the favorites of Georg Oláh, receiving his Nobel prize in chemistry for the study of carbocations, has a unique dynamical behavior which challenged standard spectroscopic models and even the best experimentalists.

We obtained detailed structural and high-resolution spectroscopic results on certain $H_xHe_n^+$ systems,[136,143, 154,161] revealing the structure and the dynamics of these unusual molecules. Some of the $H_xHe_n^+$ systems may demonstrate microscopic superfluidity,[136] a highly interesting phenomenon to study. Some other systems seem to exhibit quasistructural behavior and thus they have been in the focus of our investigations.

There have been a number of applications of the MARVEL technique to ascertain the motion of molecules and their gas-phase spectra. These studies addressed diatomic ($^{12}C_2$,[153] ^{14}NH,[139] $^{16}O_2$,[135] $^{48}Ti^{16}O$,[110] and $^{90}Zr^{16}O$[131]), triatomic (three H_2O isotopologues,[134,150,156] three $S^{16}O_2$ isotopologues (^{32}S, ^{33}S, and ^{34}S),[125] $H_2{}^{32}S$[129]), and tetratomic ($^{12}C_2H_2$,[122] NH_3,[149]) molecules, as well. In 2020 we established our W2020 database of three water isotopologues ($H_2{}^{16}O$, $H_2{}^{18}O$, and $H_2{}^{17}O$),[150,156] which is a partial update of our IUPAC database[42,52,75,85,88] of energy levels and transitions of nine water isotopologues. The improved data should help to better understand the greenhouse effect on our own planet, earth. Availability of the SO_2 data[125] is a basic requirement to understand the "great oxygenation event" (GOE), which happened some 2.5 billion years ago. Our MARVEL studies led us to be co-authors of the canonical spectroscopic database and information system of the world, HITRAN.[118]

Thermochemistry is another field of physical chemistry where detailed spectroscopic information is essential, as we have showed several times.[109,113,119] Following our related publications we became part of the TIPS (Total Internal Partition Sums) team,[119] providing thermochemical results of the highest quality to the scientific and engineering communities.

Based on our improved methodologies, we determined quasibound resonance states for a couple of polyatomic molecular systems.[116,141,151] Such studies are especially relevant for weakly-bound molecules or complexes.

Our data on heavy water[113] contributed significantly to the derivation of a new equation of state of heavy water.

Using interesting models of quantum dynamics and variational nuclear-motion computations, we investigated tunneling-type behavior and tunneling switching in several systems,[132,133] even published a review on the interesting topic of tunneling control and controlling tunneling.[158]

Community service

During the course of the grant, we involved a number of high-school students in scientific research, resulting in two publications.[135,169] Introducing high-school students to the rigor of science is an important and satisfying aspect of our research efforts, made possible by the MARVEL protocol we developed.[30,70]

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