

Tamás Szidarovszky

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WORK EXPERIENCE

Research associate

Eötvös Loránd University (ELTE) [2017 – Current]

Assistant professor

The University of Tokyo - Yamanouchi Laboratory [2016 – 2017]

JSPS postdoctoral fellow

The University of Tokyo - Yamanouchi Laboratory [2014 – 2016]

Research assistant

ELTE and MTA-ELTE Research Group on Complex Chemical Systems [2012 – 2014]

EDUCATION AND TRAINING

PhD in Theoretical Chemistry

Eötvös Loránd University (ELTE), group of Prof. Attila G. Császár [2009 – 2012]

Thesis: Rovibrational spectra near dissociation

BSc in Physics

Eötvös Loránd University (ELTE), supervisor: Dr. Zoltán Kaufmann [2009 – 2013]

Thesis: Semiclassical study of molecules (in Hungarian)

MSc in Chemistry

Eötvös Loránd University (ELTE), supervisors: Prof. Attila G. Császár and Dr. Gábor Czakó [2004 – 2009]

Thesis: Variational computation of complete molecular spectra (in Hungarian)

Short research visit

University of Arizona, AZ, USA, group of Prof. Árpád Somogyi [2008]

Field(s) of study: Automatization of mass spectra analysis

Short research visit

University of Arizona, AZ, USA, group of Prof. Árpád Somogyi [2006]

Field(s) of study: Investigating the tholin-water reaction using high-resolution mass spectrometry

PUBLICATIONS

2020

- (40) Spectroscopic signatures of HHe₂[±] and HHe₃[±]
- M. Töpfer, A. Jensen, K. Nagamori, H. Kohguchi, T. Szidarovsky, A. G. Császár, S. Schlemmer and O. Asvany *Phys. Chem. Phys. accepted for publication*.
- (39) Rotational-vibrational resonance states
- A. G. Császár, I. Simkó, T. Szidarovszky, G. C. Groenenboom, T. Karman and Ad van der Avoird *Phys. Chem. Phys.*, **22**, 15081-15104 (2020).
- (38) Three-player polaritons: nonadiabatic fingerprints in an entangled atom-molecule-photon system
- T. Szidarovszky, G. J. Halász and Á. Vibók New J. Phys. 22, 053001 (2020).
- (37) Robust field-dressed spectra of diatomics in an optical lattice
- M. Pawlak, T. Szidarovszky, G. J. Halász and Á. Vibók Phys. Chem. Chem. Phys. 22, 3715-3723 (2020).
- (36) Excited-state populations in the multiconfiguration time-dependent Hartree-Fock method
- E. Lötstedt, T. Szidarovszky, F. H. M. Faisal, T. Kato and K. Yamanouchi J. Phys. B, 53, 105601 (2020).

2019

- (35) Infrared signatures of the HHe_n $^{\pm}$ and DHe_n $^{\pm}$, n = 3-6, complexes
- O. Asvany, S. Schlemmer, T. Szidarovszky and A. G. Császár J. Phys. Chem. Lett. 10, 5325-5330 (2019).
- (34) Rovibronic spectra of molecules dressed by light fields
- T. Szidarovszky, A. G. Császár, G. J. Halász and Á. Vibók Phys. Rev. A 100, 033414 (2019).
- (33) Toward automated variational computation of rovibrational resonances. A case study of the H₂ dimer
- I. Simkó, T. Szidarovszky and A. G. Császár J. Chem. Theory Comput. 15, 4156-4169 (2019).
- (32) Fingerprints of microscopic superfluidity in HHe_n[±] clusters
- A. G. Császár, T. Szidarovszky, O. Asvany and S. Schlemmer Mol. Phys. 117, 1559-1583 (2019).

2018

- (31) Conical intersections induced by quantum light: field-dressed spectra from the weak to the ultrastrong coupling regimes
- T. Szidarovszky, G. J. Halász, A. G. Császár, Lorenz S. Cederbaum and Á. Vibók *J. Phys. Chem. Lett.* 9, 6215-6223 (2018).
- (30) Direct signatures of light-induced conical intersections on the field-dressed spectrum of Na₂
- T. Szidarovszky, G. J. Halász, A. G. Császár, Lorenz S. Cederbaum and Á. Vibók *J. Phys. Chem. Lett.* 9, 2739-2745 (2018).
- (29) Rovibrational resonances in H₂He[±]
- D. Papp, A. G. Császár, K. Yamanouchi and T. Szidarovszky, J. Chem. Theory Comput. 14, 1523-1533 (2018).
- (28) <u>LIMAO: Cross-platform software for simulating laser-induced alignment and orientation dynamics of linear-, symmetric- and asymmetric tops</u>
- T. Szidarovszky, M. Jono and K. Yamanouchi, Comput. Phys. Commun. 228, 219-228 (2018).

- (27) A general variational approach for computing rovibrational resonances of polyatomic molecules. Application to the weakly bound H_2He^\pm and $H_2\cdot CO$ systems
- D. Papp, T. Szidarovszky and A. G. Császár, J. Chem. Phys. 147, 094106 (2017).
- (26) Recommended ideal-gas thermochemical functions for heavy water and its substituent isotopologues
- I. Simkó, T. Furtenbacher, J. Hrubý, N. F. Zobov, O. L. Polyansky, J. Tennyson, R. R. Gamache, T. Szidarovszky, N. Dénes and A. G. Császár, *J. Phys. Chem. Ref. Data* 46, 023104 (2017).
- (25) Full-dimensional simulation of the laser-induced alignment dynamics of H₂He[±]
- T. Szidarovszky and K. Yamanouchi, Mol. Phys. (André D. Bandrauk Special Issue) 115, 1916-1926 (2017).
- (24) Complex rovibrational dynamics of the Ar-NO[±] complex
- D. Papp, T. Szidarovszky, J. Sarka, E. Mátyus, A. G. Császár, M. Hochlaf and T. Stoecklin, *Phys. Chem. Chem. Phys.* 19, 8152-8160 (2017).

2016

- (23) Photodissociation dynamics of weakly bound HeH₂[±] in intense light fields
- T. Szidarovszky and K. Yamanouchi, Phys. Rev. A 94, 063405 (2016).
- (22) Definitive ideal-gas thermochemical functions of the $H_2^{16}O$ molecule
- T. Furtenbacher, T. Szidarovszky, J. Hrubý, A. A. Kyuberis, N. F. Zobov, O. L. Polyansky, J. Tennyson and A. G. Császár, *J. Phys. Chem. Ref. Data* 45, 043104, (2016).
- (21) Fragmentation of long-lived hydrocarbons after strong field ionization
- S. Larimian, S. Erattupuzha, E. Lötstedt, T. Szidarovszky, R. Maurer, S. Roither, M. Schöffler, D. Kartashov, A. Baltuška, K. Yamanouchi, M. Kitzler and X. Xie, *Phys. Rev. A* 93, 053405 (2016).

2015

- (20) Modelling rotations, vibrations, and rovibrational couplings in astructural molecules a case study based on the H_5^{\pm} molecular ion
- J. Sarka, C. Fábri, T. Szidarovszky, A. G. Császár, Z. Lin and A. B. McCoy, Mol. Phys. 113, 1873-1883 (2015).
- (19) <u>Toward accurate thermochemistry of the ²⁴MgH, ²⁵MgH, and ²⁶MgH molecules at elevated temperatures: corrections due to unbound states</u>
- T. Szidarovszky and A. G. Császár, J. Chem. Phys. 142, 014103 (2015).

2014

- (18) Modelling non-adiabatic effects in $H_{\underline{3}^{\pm}}$: solution of the rovibrational Schrödinger equation with motion-dependent masses and mass surfaces
- E. Mátyus, T. Szidarovszky and A. G. Császár, J. Chem. Phys. 141, 154111 (2014).
- (17) Grid-based empirical improvement of molecular potential energy surfaces
- T. Szidarovszky and A. G. Császár, J. Phys. Chem. A 118, 6256-6265 (2014).
- (16) <u>IUPAC critical evaluation of the rotational-vibrational spectra of water vapor. Part IV. Energy levels and transition wavenumbers for $D_2^{16}O$, $D_2^{17}O$, and $D_2^{18}O$ </u>
- J. Tennyson, P. F. Bernath, L. R. Brown, A. Campargue, A. G. Császár, L. Daumont, R. R. Gamache, J. T. Hodges, O. V. Naumenko, O. L. Polyansky, L. S. Rothman, A. C. Vandaele, N. F. Zobov, N. Dénes, A. Z. Fazliev, T. Furtenbacher, I. E. Gordon, S.-M. Hu, T. Szidarovszky and I. A. Vasilenko, *J. Quant. Spectr. Rad. Transfer* 142, 93-108 (2014).

- (15) Analysis of the rotational-vibrational states of the molecular ion H₃[±]
- T. Furtenbacher, T. Szidarovszky, E. Mátyus, C. Fábri and A. G. Császár, *J. Chem. Theory Comput.* 9, 5471-5478 (2013).
- (14) Low-lying quasibound rovibrational states of H₂¹⁶O
- T. Szidarovszky and A. G. Császár, Mol. Phys. (Martin Quack Special Issue) 111(14-15), 2131-2146 (2013).
- (13) MARVEL analysis of the rotational-vibrational states of the molecular ions H₂D[±] and D₂H[±]
- T. Furtenbacher, T. Szidarovszky, C. Fábri and A. G. Császár, *Phys. Chem. Chem. Phys. (Themed Issue on Spectroscopy and Dynamics of Medium-Sized Molecules and Clusters)* 15, 10181-10193 (2013).

2012

- (12) Molecular structure and dynamics (in Hungarian)
- A. G. Császár, G. Czakó, T. Furtenbacher, E. Mátyus, C. Fábri, T. Szidarovszky, I. Szabó and J. Sarka, *Magy. Kem. Foly.* 118, 181-189 (2012).
- (11) <u>Precision measurements and computations of transition energies in rotationally cold triatomic hydrogen ions up to the mid-visible spectral range</u>
- M. Pavanello, L. Adamowicz, A. Alijah, N. F. Zobov, I. I. Mizus, O. L. Polyansky, J. Tennyson, T. Szidarovszky, A. G. Császár, M. Berg, A. Petrignani, A. Wolf, *Phys. Rev. Lett.* 108, 023002 (2012).
- (10) Calibration-quality adiabatic potential energy surfaces for H₃[±] and its isotopologues
- M. Pavanello, L. Adamowicz, A. Alijah, N. F. Zobov, I. I. Mizus, O. L. Polyansky, J. Tennyson, T. Szidarovszky and A. G. Császár, *J. Chem. Phys.* 136, 184303 (2012).
- (9) The role of axis embedding on rigid rotor decomposition (RRD) analysis of variational rovibrational wave functions
- T. Szidarovszky, C. Fábri and A. G. Császár, J. Chem. Phys. 136, 174112 (2012).
- (8) A Paradox of grid-based representation techniques: accurate eigenvalues from inaccurate matrix elements
- V. Szalay, T. Szidarovszky, G. Czakó and A. G. Császár, J. Math. Chem. 50, 636-651 (2012).
- (7) Spectroscopy of H₃[±] based on a new high accuracy global potential energy surface
- O. L. Polyansky, A. Alijah, N. F. Zobov, I. I. Mizus, R. I. Ovsyannikov, J. Tennyson, L. Lodi, T. Szidarovszky and A. O. Orforfy, Phil. Trans. B. Cos. A 970, 5014 5007 (2010).
- G. Császár, Phil. Trans. R. Soc. A 370, 5014-5027 (2012).
- (6) The fourth age of quantum chemistry: molecules in motion
- A. G. Császár, C. Fábri, T. Szidarovszky, E. Mátyus, T. Furtenbacher and G. Czakó, *Phys. Chem. Chem. Phys.* 14(3), 1085-1106 (2012).

2011

- (5) <u>Gas-phase and Ar-matrix SQM scaling factors for various DFT functionals with basis sets including</u> polarization and diffuse functions
- C. Fábri, T. Szidarovszky, G. Magyarfalvi and Gy. Tarczay, J. Phys. Chem. A 115 (18), 4640-4649 (2011).

2010

- (4) Assigning quantum labels to variationally computed rotational-vibrational eigenstates of polyatomic molecules
- E. Mátyus, C. Fábri, T. Szidarovszky, G. Czakó, W. D. Allen and A. G. Császár, *J. Chem. Phys.* 133, 034113 (2010).
- (3) On the efficiency of treating singularities in triatomic variational vibrational computations. The vibrational states of H_3^{\pm} up to dissociation
- T. Szidarovszky, A. G. Császár and G. Czakó, Phys. Chem. Chem. Phys. 12, 8373-8386 (2010).
- (2) First-principles prediction and partial characterization of the vibrational states of water up to dissociation
- A. G. Császár, E. Mátyus, T. Szidarovszky, L. Lodi, N. F. Zobov, S. V. Shirin, O. L.Polyansky and J. Tennyson, *J. Quant. Spectr. Rad. Transfer* 111(9), 1043-1064 (2010).

2009

(1) Conformers of gaseous threonine

T. Szidarovszky, G. Czakó and A. G. Császár, *Mol. Phys. (Henry F. Schaefer Special Issue)* 107(8-12), 761-775 (2009).

Book chapters

- (B3) Exact numerical methods for stationary-state-based quantum dynamics of complex polyatomic molecules
- A. G. Császár, C. Fábri, T. Szidarovszky, in *Molecular Spectroscopy and Quantum Dynamics*, in press.
- (B2) <u>Light-dressed spectroscopy of molecules</u>
- T. Szidarovszky, A. G. Császár, G. J. Halász, Á. Vibók, in *Progress in Ultrafast Intense Laser Science* volume XV, chapter 4.
- (B1) Laser-induced alignment and orientation dynamics beyond the rigid-rotor approximation
- T. Szidarovszky, K. Yamanouchi, in *Progress in Ultrafast Intense Laser Science* volume XIV, chapter 2.

List of publications available on

Google Scholar, Publons, Scopus or on the Hungarian Scientific Bibliography

FELLOWSHIPS, PRIZES

Prizes

- Academic Youth Prize (Hungarian Academy of Sciences, 2020)
- o 'Excellent researcher of the Institute' (Institute of Chemistry, Eötvös Loránd University, 2019)
- o 'Excellent student of the Faculty' (Faculty of Sciences, Eötvös Loránd University, 2007)

Fellowships

- o FK20 Grant (NKFIH Young Researcher Excellence Program, 2020 2024)
- o Bolyai+ Young Researcher Fellowship (New National Excellence Program, 2020)
- o Bolyai János Research Fellowship (Hungarian Academy of Sciences, 2020 2023)
- PD17 Fellowship (NKFIH Postdoctoral Excellence Program, 2017 2020)
- JSPS Postdoctoral Fellowship (Japan Society for the Promotion of Science, 2014 2016)
- o Erdős Pál Young Researcher Fellowship (National Excellence Program, 2014)
- o Scholarship of the Hungarian Republic (2007 2008)

COMMUNITY SERVICE

Member, Reviewer Board (Photonics, MDPI)

[2020 - Current]

Member, public body of the Hungarian Academy of Sciences

[2018 - Current]

AMMB Working Committee, Committee on Physical Chemistry, Section of Chemical Sciences

Science communication

- Presenter at Turbine Academy (Budapest, Hungary, 2019)
- Finalist of FameLab Hungary (Hungarian Academy of Sciences, 2019)
- o Science Dialogue presenter (Hikawa Highshcool, Yamanashi, Japan, 2015)
- Presenter at AtomCsill (Eötvös Loránd University, Institute of Physics, 2013)