

## PERSONAL INFORMATION



## Tamás Szidarovszky

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## WORK EXPERIENCE

2017–Present

## Research associate

**Eötvös Loránd University (ELTE)**

Laboratory of Molecular Structure and Dynamics

**Hungarian Academy of Sciences (MTA)**

MTA-ELTE Research Group on Complex Chemical Systems

2016–2017

## Assistant professor

**The University of Tokyo**

Yamanouchi Laboratory -Molecules in Intense Laser Fields-

2014–2016

## JSPS postdoctoral fellow

**The University of Tokyo**

Yamanouchi Laboratory -Molecules in Intense Laser Fields-

2012–2014

## Research assistant

**Eötvös Loránd University (ELTE)**

Laboratory of Molecular Structure and Dynamics

**Hungarian Academy of Sciences (MTA)**

MTA-ELTE Research Group on Complex Chemical Systems

## EDUCATION AND TRAINING

2009–2012

## PhD in Theoretical Chemistry

**Eötvös Loránd University (ELTE)**, group of Prof. Attila G. Császár

*Thesis: Rovibrational spectra near dissociation*

2009–2013

## BSc in Physics

**Eötvös Loránd University (ELTE)**, supervisor: Dr. Zoltán Kaufmann

*BSc Thesis: Semiclassical study of molecules (in Hungarian)*

2004–2009

## MSc in Chemistry

**Eötvös Loránd University (ELTE)**, supervisors: Prof. Attila G. Császár and Dr. Gábor Czakó

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

2008

## Short research visit

**University of Arizona, AZ, USA**, group of Prof. Árpád Somogyi

*Research topic: Automatization of mass spectra analysis*

2006

## Short research visit

**University of Arizona, AZ, USA**, group of Prof. Árpád Somogyi

*Research topic: Investigating the tholin-water reaction using high-resolution mass spectrometry*

## PERSONAL SKILLS

Mother tongue(s) Hungarian

Foreign language(s)

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
English	C2	C2	C1	C2	C2
German	A1	A1	A1	A1	A1
Japanese	A1	A1	A1	A1	

Levels: A1 and A2: Basic user - B1 and B2: Independent user - C1 and C2: Proficient user  
Common European Framework of Reference for Languages

## ADDITIONAL INFORMATION

Fellowships, prizes

- 'Excellent researcher of the Institute' (Institute of Chemistry, Eötvös Loránd University) (2019)
- PD\_17 Fellowship (NKFIH Postdoctoral Excellence Program) (2017-2020)
- JSPS (Japan Society for the Promotion of Science) Postdoctoral Fellowship (2014 - 2016)
- Erdős Pál Young Researcher Fellowship (National Excellence Program) (2014)
- Scholarship of the Hungarian Republic (2007 - 2008)
- 'Excellent student of the Faculty' (Faculty of Sciences, Eötvös Loránd University) (2007)

Personal

- Born in Budapest, Hungary 1985.09.06
- Parents are Dr. Gabriella Szép and Dr. Ferenc Szidarovszky
- Married to Alexandra Urbán

Publications

## Research articles

## 2019

- (37) Robust field-dressed spectra of diatomics in an optical lattice  
M. Pawlak, T. Szidarovszky, G. J. Halász, Á. Vibók *Phys. Rev. A*, submitted.
- (36) Infrared signatures of the  $\text{HHe}_n^+$  and  $\text{DHe}_n^+$ ,  $n = 3-6$ , complexes  
O. Asvany, S. Schlemmer, T. Szidarovszky, A. G. Császár *J. Phys. Chem. Lett.*, submitted
- (35) Excited-state populations in the multiconfiguration time-dependent Hartree-Fock method  
E. Lötstedt, T. Szidarovszky, F. H. M. Faisal, T. Kato, K. Yamanouchi *Phys. Rev. A*, submitted.
- (34) Rovibronic spectra of molecules dressed by light fields  
T. Szidarovszky, A. G. Császár, G. J. Halász, Á. Vibók *Phys. Rev. A*, submitted.
- (33) Toward automated variational computation of rovibrational resonances. A case study of the  $\text{H}_2$  dimer  
I. Simkó, T. Szidarovszky, A. G. Császár *J. Chem. Theory Comput.*, in press.
- (32) Fingerprints of microscopic superfluidity in  $\text{HHe}_n^+$  clusters  
A. G. Császár, T. Szidarovszky, O. Asvany, S. Schlemmer *Mol. Phys.* 117, 1559 (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, Á. Vibók *J. Phys. Chem. Lett.* 9, 6215 (2018).
- (30) Direct signatures of light-induced conical intersections on the field-dressed spectrum of  $\text{Na}_2$   
T. Szidarovszky, G. J. Halász, A. G. Császár, Lorenz S. Cederbaum, Á. Vibók *J. Phys. Chem. Lett.* 9, 2739 (2018).
- (29) Rovibrational resonances in  $\text{H}_2\text{He}^+$   
D. Papp, A. G. Császár, K. Yamanouchi, T. Szidarovszky, *J. Chem. Theory Comput.* 14, 1523 (2018).

(28) LIMAO: Cross-platform software for simulating laser-induced alignment and orientation dynamics of linear-, symmetric- and asymmetric tops

T. Szidarovszky, M. Jono, K. Yamanouchi, *Comput. Phys. Commun.* 228, 219 (2018).

## 2017

(27) A general variational approach for computing rovibrational resonances of polyatomic molecules. Application to the weakly bound  $\text{H}_2\text{He}^+$  and  $\text{H}_2\text{-CO}$  systems

D. Papp, T. Szidarovszky, 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  $\text{H}_2\text{He}^+$

T. Szidarovszky and K. Yamanouchi, *Mol. Phys. (André D. Bandrauk Special Issue)* 115, 1916 (2017).

(24) Complex rovibrational dynamics of the  $\text{Ar-NO}^+$  complex

D. Papp, T. Szidarovszky, J. Sarka, E. Mátyus, A. G. Császár, M. Hochlaf and T. Stoecklin, *Phys. Chem. Chem. Phys.* 19, 8152 (2017).

## 2016

(23) Photodissociation dynamics of weakly bound  $\text{HeH}_2^+$  in intense light fields

T. Szidarovszky and K. Yamanouchi, *Phys. Rev. A* 94, 063405 (2016).

(22) Definitive ideal-gas thermochemical functions of the  $\text{H}_2^{16}\text{O}$  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 a structural molecules - a case study based on the  $\text{H}_5^+$  molecular ion

J. Sarka, C. Fábri, T. Szidarovszky, A. G. Császár, Z. Lin and A. B. McCoy, *Mol. Phys.* 113, 1873 (2015).

(19) Toward accurate thermochemistry of the  $^{24}\text{MgH}$ ,  $^{25}\text{MgH}$ , and  $^{26}\text{MgH}$  molecules at elevated temperatures: corrections due to unbound states

T. Szidarovszky and A. G. Császár, *J. Chem. Phys.* 142, 014103 (2015).

## 2014

(18) Modelling non-adiabatic effects in  $\text{H}_3^+$ : 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) IUPAC critical evaluation of the rotational-vibrational spectra of water vapor. Part IV. Energy levels and transition wavenumbers for  $\text{D}_2^{16}\text{O}$ ,  $\text{D}_2^{17}\text{O}$ , and  $\text{D}_2^{18}\text{O}$

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).

## 2013

(15) Analysis of the rotational-vibrational states of the molecular ion  $\text{H}_3^+$

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  $\text{H}_2^{16}\text{O}$

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  $\text{H}_2\text{D}^+$  and  $\text{D}_2\text{H}^+$

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) Spectroscopy of $H_3^+$ 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. G. Császár, *Phil. Trans. R. Soc. A* 370, 5014-5027 (2012).

### (10) Calibration-quality adiabatic potential energy surfaces for $H_3^+$ 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) Precision measurements and computations of transition energies in rotationally cold triatomic hydrogen ions up to the mid-visible spectral range

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. Petignani, A. Wolf, *Phys. Rev. Lett.* 108, 023002 (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) Gas-phase and Ar-matrix SQM scaling factors for various DFT functionals with basis sets including 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 $H_3^+$ 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

## 2019

### (3) 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*, submitted.

### (2) Light-dressed spectroscopy

T. Szidarovszky, A. G. Császár, G. J. Halász, Á. Vibók, in *Progress in Ultrafast Intense Laser Science* volume XV, submitted.

### (1) Laser-induced alignment and orientation dynamics beyond the rigid-rotor approximation

T. Szidarovszky, K. Yamanouchi, in *Progress in Ultrafast Intense Laser Science* volume XIV, chap. 2.