Curriculum vitae: **PUSZTAI, László** György

Born: 07 June 1963 (Szeged, Hungary)
Marital status: married (3 children)

Contact details
Wigner Research Centre for Physics, H-1121 Budapest, Konkoly Thege út 29-33.
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Academic qualifications
Doctor of the Hungarian Academy of Sciences (D.Sc.), April 2000: Title of Theses: 'Inverse methods for the interpretation of (liquid- and amorphous-) diffraction data'
Candidate of Sciences, January 1992 (Ph.D. issued by the Hungarian Academy of Sciences; closest equivalent is Ph.D.): Title of Thesis: 'Investigation of disordered structures by Reverse Monte Carlo simulation'.
Diploma in Chemistry, July 1987: Awarded first class diploma in Chemistry by L. Eötvös Univ., Budapest, Hungary. (Closest equivalent is M. Sc.)

Research experience
1 April 2017 –
Distinguished Professor (part time) at the International Research Organization for Advanceed Science and Technology (IROAST), Kumamoto University, Japan.
1 February 1999 -
Scientific advisor (until 31 December 2016: leader, 'Liquid structure group'; until 1 January 2013: Head, Neutron Physics Laboratory), at the Institute for Solid State Physics and Optics, Wigner Research Centre for Physics (until 31 August 2019: of the Hungarian Academy of Sciences; until 31 December 2011: Institute for Solid State Physics and Optics, Hungarian Academy of Sciences). Neutron and X-ray scattering investigations of disordered materials (mostly molecular liquids and solids). Further development of the Reverse Monte Carlo technique.
September 1991 - January 1999
Research fellow at the Laboratory of Theoretical Chemistry, L. Eötvös University. Research on the methodology of the Reverse Monte Carlo simulation and its applications, mainly for glassy materials and molecular liquids, including water.
September 1995 - January 1998
Post doctoral fellow at Studsvik NFL (University of Uppsala, Sweden). Research on MCGR

('Monte Carlo analysis for obtaining G of R') and Reverse Monte Carlo (RMC) for neutron diffraction data analysis. Neutron diffraction experiments on liquid and solid CX_4 (X=Cl, Br, I) compounds.

June 1992 - November 1992

Research fellow at the Laboratory of Materials Science, Delft University of Technology (funded by: TU Delft). Research work on the structure of metallic glasses.

July 1990-November 1990

Visitor at Clarendon Laboratory, University of Oxford, funded by 'Széchenyi István Scholarship Foundation', Budapest. Studies of different disordered structures, such as metallic glasses and liquid and amorphous monatomic systems.

September 1988-September 1991

Research student at the Laboratory of Theoretical Chemistry, Loránd Eötvös University, Budapest, funded by the Hungarian Academy of Sciences. Title of project: 'Studies of liquid structures by computer simulation methods'.

October 1987-July 1988

Visiting graduate student at Keble College, University of Oxford. Research at the Clarendon Laboratory; development of the Reverse Monte Carlo method (with Prof. R.L. McGreevy).

Guest researcher: University of Kent at Canterbury, UK (1995, 2 months); Universite de Bordeaux I, France (2001, 3 months); Universidad Nacional Autonoma de Mexico (2003, 3 months); Maria Sklodowska University, Lublin, Poland (2008, 2 months); JSPS Guest Senior Research Fellow, SPring-8, Japan (2010, 3 weeks).

Publications

About 165 research papers and book chapters in international scientific journals. One book titled ‘Disorder in condensed phases’ (in Hungarian; Akadémiai Kiadó, 1995, Budapest). About 3600 independent citations (as of 05 March 2021). 30 invited talks over the past 10 years (about 40 altogether).

List of publications, László Pusztai

(IF: impact factor of journal)

Research papers

1) L Pusztai, A Baranyai and I Ruff, 'Vacancies in molten salts: A characteristic feature of the structure', *J. Phys. C: Solid State Phys*. **21**, 3687 (1988) IF: 1.98

2) A Baranyai, L Pusztai and I Ruff, 'Second order invariants of spherical harmonics as order parameters in disordered systems', *Electrochimica Acta* **33**, 1229 (1988) IF: 1.19

3) RL McGreevy and L Pusztai, 'Reverse Monte Carlo simulation: A new technique for the determination of disordered structures', *Mol.Sim*. **1**, 359 (1988) https://doi.org/10.1080/08927028808080958 IF: 1.38

4) L Pusztai and RL McGreevy, 'Vacancy dynamics in molten RbCl', *Phys. Chem. Liq*. **19**, 63 (1989) IF: 0.74

5) L Pusztai and RL McGreevy, 'Dynamics of molten alkali halides: LiCl and KCl', *J. Phys.: Cond. Matt.* **1**, 2369 (1989) IF: 2.41

6) RL McGreevy and L Pusztai, 'The structure of molten salts', *Proc. Roy. Soc. Lond. A* **430**, 241 (1990) IF: 1.55

7) L Pusztai and RL McGreevy, 'The structure of glassy zinc chloride: A Reverse Monte Carlo study', *J. Non-Cryst. Sol*. **117-118**, 627 (1990) IF: 1.02

8) L Pusztai, 'Modelling of partial and total radial distribution functions of amorphous Ni_2B using Reverse Monte Carlo Simulation', *Z. Naturf. 46a*, **69** (1991) IF: 0.70

9) L Pusztai and G Tóth, 'On the uniqueness of the Reverse Monte Carlo simulation: 1. Simple liquids, partial radial distribution functions', *J. Chem. Phys*. **94**, 3042 (1991) IF: 3.57

10) L Pusztai and RL McGreevy, 'The structure of liquid and superfluid ^{4}He across the □-point', *Phys. Chem Liq.* **24** 119 (1991) IF: 0.46

SUM1988_1991=15

11) G Tóth and L Pusztai, 'Comparative studies of the underlying local order corresponding to different radial distributions of disordered systems', *Chem. Phys*. **160**, 405 (1992) IF: 1.96

12) G Tóth and L Pusztai, 'Determination of the radial distribution function of small particle polymer latices using Reverse Monte Carlo Simulation' , *J. Phys. Chem*. **96**, 7150 (1992) IF: 3.45

13) G Tóth and L Pusztai, 'Determination of effective hard core diameters of liquids from their static vacancy distributions', *Z. Phys. Chem*. **178**, 55 (1992) IF: 0.68

14) EW Iparraguirre, J Sietsma, BJ Thijsse and L Pusztai, ' A Reverse Monte Carlo study of amorphous $Ni_{81}B_{19}$', *Computational Materials Science* **1**, 110 (1993) IF: 0.67

15) L Pusztai and E Sváb, 'Structure study of $Ni_{62}Nb_{38}$ metallic glass using Reverse Monte Carlo simulation', *J. Non-Cryst. Sol*. **156-158**, 973 (1993) IF: 0.97

16) MA Howe, RL McGreevy, L Pusztai and I Borzsák', Determination of 3 body correlations in simple liquids by RMC modelling of diffraction data. 2. Elemental liquids', *Phys. Chem. Liq*. **25**, 205 (1993) IF: 0.40

17) S Kugler, L Pusztai, L Rosta, R Bellisent and P Chieux, 'The structure of evaporated pure amorphous silicon: Neutron diffraction and Reverse Monte Carlo investigations', *Phys. Rev. B* **48**, 7685 (1993) IF: 3.16

18) L Pusztai and S Kugler, 'Reverse Monte Carlo simulation: The structure of amorphous silicon', *J. Non-Cryst. Sol*. **164-166**, 147 (1993) IF: 0.97

[Short version: S Kugler and L Pusztai, `Investigations on the structure of evaporated pure amorphous silicon', *Acta Physica Hungarica* **75**, 261 (1994)]

19) L Pusztai and E Sváb, 'Modelling the structure of $Ni_{65}B_{35}$ metallic glass by Reverse Monte Carlo simulation', *J. Phys: Cond. Mat*., **5**, 8815 (1993) IF: 1.65

20) OA Pizio and L Pusztai, 'Triplet correlations in the molten phase of Ag_2Se superionic conductor', *Chem. Phys. Lett.,* **214**, 125 (1993) IF: 3.02

SUM1992_1993=16.93

21) PA Duine, L Pusztai and J Sietsma, 'A search for static-structure changes in disordered systems in connection with atomic-mobility changes', *Mat. Sci. Eng*. **A178**, 279 (1994) IF: 0.99

22) L Pusztai and O Gereben, 'On the determination of the structure of metallic glasses by Reverse Monte Carlo simulation: Comparison with hard sphere Monte Carlo results', *Mat. Sci. Eng*. **A179/180**, 433 (1994) IF: 0.99

23) O Gereben, L Pusztai and A Baranyai, 'Calculation of the three-particle contribution to the configurational entropy for two different models of amorphous Si', *Phys. Rev. B* **49**, 13251 (1994) IF: 3.19

24) G Petõ, Zs Horváth, O Gereben, L Pusztai, F Hajdú and E Sváb, 'Implantation-induced structural changes in evaporated amorphous Ge', *Phys. Rev. B* **50**, 539 (1994) IF: 3.19

25) O Gereben and L Pusztai, `Structure of amorphous semiconductors: Reverse Monte Carlo studies on a-C, a-Si and a-Ge', *Phys. Rev. B,* **50**, 14136 (1994) IF: 3.19

26) PA Duine, J Sietsma, BJ Thijsse and L Pusztai, `A Reverse Monte Carlo study of structure changes in amorphous $Pd_{52}Ni_{32}P_{16}$ upon annealing', *Phys. Rev. B*, **50**, 13240 (1994) IF: 3.19

27) O Gereben, L Pusztai and A Baranyai, `Possible quantitative measures of order/disorder in models of liquid and amorphous structures', *J. Phys.: Condensed Matter*, **6**, 10939 (1994) IF: 1.56

28) L Pusztai, O Gereben and A Baranyai, `Some remarks on the measured structure factor', *Physica Scripta*, **T57**, 69 (1994) IF: 0.99

29) L Pusztai, J Sietsma and BJ Thijsse, `Structure and relaxation of the metallic glass $Pd_{52}Ni_{32}P_{16}$ modelled by Reverse Monte Carlo simulation', *Phil Mag. B*, **71**, 383 (1995) IF: 1.23

30) O Gereben and L Pusztai, `Determination of the microscopic structure of disordered materials on the basis of limited Q-space information', *Phys. Rev. B* **51**, 5768 (1995)
[Short version: L Pusztai and O Gereben, `Pair correlation functions obtained from very short structure factors, using Reverse Monte Carlo', *Acta Physica Hungarica* **75**, 257 (1994)]
IF: 2.83

31) L Pusztai, `Partial pair correlation functions of some Ge-Sb Liquid alloys from single diffraction measurements', *ACH -- Models in Chemistry* **132**, 99 (1995) IF: 0.39

32) L Pusztai and O Gereben, `Reverse Monte Carlo approach to the structure of amorphous semiconductors', *J. Non-Cryst. Solids* **192-193**, 640-643 (1995) IF: 1.13
SUM1994_1995=22.87

33) O Gereben and L Pusztai, `The determination of the microscopic density in liquids and other disordered materials using Reverse Monte Carlo simulation', *Phys. Chem. Liquids* **31**, 159 (1996) IF: 0.31

34) RL McGreevy and L Pusztai, `Assessing the relative information content of different types of diffraction measurements for liquids and glasses', *J. Neutron Research* **3**, 125 (1996) IF: ???

35) O Gereben and L Pusztai, `The like-like-like partial triplet correlation functions of amorphous $Ni_{62}Nb_{38}$', *J. Non-Cryst. Solids*, **205-207**, 716 (1996) IF: 1.13

36) L Pusztai and RJ Newport, `Reverse Monte Carlo model calculations on a-C:H two-component systems', *Z. Phys. B*, **101**, 631 (1996) IF: 1.65

37) L Pusztai and RL McGreevy, `The structure of liquid CCl_4', *Molec. Phys*., **90**, 533 (1997) IF: 1.70

38) L Pusztai and RL McGreevy,`MCGR: an inverse method for deriving the pair correlation function from the structure factor', *Physica B* **234-236**, 357 (1997) IF: 0.99

39) L Pusztai and RL McGreevy, 'The structure of molten CuBr', *J. Phys.: Condensed Matter* **10***,* 525 (1998) IF: 1.65

40) L Pusztai, 'Structural modelling using the reverse Monte Carlo technique: Application to amorphous semiconductors', *J. Non-Cryst. Sol.* **227-230**, 88 (1998) IF: 1.06

41) RL McGreevy and L. Pusztai, 'RMC modelling methods for polymers and polymer electrolytes: progress, problems and prospects', *Electrochimica Acta* **43**, 1349 (1998) IF: 1.52

SUM1996-1998=10.01

42) G. Tóth, L. Pusztai, A. Baranyai, 'Comment on: A new algorithm for Reverse Monte Carlo simulations [J. Chem. Phys. 109, 2634 (1998)]', *J. Chem. Phys*. **111,** 5620 (1999) IF: 3.29

43) L. Pusztai, 'On the partial pair correlation functions of liquid water', *Phys. Rev. B* **60,** 11851 (1999) IF: 3.01

44) L Pusztai, RL McGreevy, 'MCGR: an Inverse Method for Deriving the Pair Correlation Function', *J. Neutron Res.* **8,** 17 (1999) IF: ???

45) L. Pusztai, 'On the structure of high and low density amorphous ice', *Phys. Rev. B* **61,** 28 (2000 January) IF: 3.07

46) L. Pusztai, `Comparison between the structures of liquid water and (high and low density) amorphous ice', *PCCP* **2**, 2703 (2000 May) IF: 1.65

47) L. Pusztai, 'How well do we know the structure of liquid water?', *Physica B* **276-278,** 419 (2000) IF: 0.89

48) P. Jóvári, Gy. Mészáros, L. Pusztai, L. Sváb, 'Neutron diffraction studies on liquid CCl_4 and C_2Cl_4', *Phyica B* **276-278**, 491 (2000) IF: 0.89

SUM1999_2000=12.8; SUM1987-2000=77.61

49) P. Jóvári, Gy. Mészáros, L. Pusztai, L. Sváb, 'The structure of liquid tetrachlorides CCl_4, $SiCl_4$, $GeCl_4$, $TiCl_4$, VCl_4 and $SnCl_4$', *J. Chem. Phys*. **114**, 8082 (2001 May) IF: 3.15

50) P. Jóvári, L. Pusztai, 'Structure of disordered forms of selenium close to the melting point', *Phys. Rev. B* **64**, 014205 (2001 June) IF: 3.07

51) L. Pusztai, R.L. McGreevy, 'The structure of molten $ZnCl_2$ and $MgCl_2$', *J. Phys.: Condens. Matter* **13**, 7213 (2001 August) IF: 1.70

52) L. Pusztai, 'Further notes concerning the partial pair correlation functions of liquid (ambient) water', *Physica A* **314**, 514-520 (2002 August) IF: 1.37

53) L. Pusztai, H. Dominguez, O.A. Pizio, 'Reverse Monte Carlo simulation of the microscopic structure for chemically associating fluids by using experimental data', *Physica A* **316**, 65-76 (2002) IF: 1.37

54) P. Jóvári, L. Pusztai, 'On the structure of red amorphous phosphorus', *Appl. Phys. A*, **74** [Suppl.], S1092-S1094 (2002) IF: 2.23

55) P. Jóvári, Gy. Mészáros, L. Pusztai, E. Sváb, 'Neutron diffraction studies of some simple molecular systems: Si_2Cl_6, CBr_3D and CD_3I', *Appl. Phys. A*, , **74** [Suppl.], S1354-S1356 (2002) IF: 2.23

SUM2001_2002=15.12

56) L. Pusztai, J.-C. Soetens, P.A. Bopp, 'The static dielectric constant and molecular geometries in ambient water studied by reverse Monte Carlo simulations', *Physica A* **323**, 42-50 (2003 April) IF: 1.18

57) P. Jóvári, R.G. Delaplane, L. Pusztai, 'Structural models of amorphous selenium', *Phys. Rev. B* **67**, 172201(-1-4) (2003 May) IF: 2.96

58) A. Patrykiejew, O. Pizio, L. Pusztai, S. Sokolowski, 'Effects of slit-like pore confinement on the closed loop immiscibility in symmetric binary model mixtures: fundamental measure density functional approach', *Mol. Phys.* **101**, 2219-2223 (2003) IF: 1.59

59) S. Kugler, K. Kohary, K. Kádas, L. Pusztai, 'Unusual atomic arrangements in amorphous silicon', *Sol. St. Comm*. **127**, 305-309 (2003 June) IF: 1.60

60) L. Pusztai, H. Dominguez, O.A. Pizio, 'The structure of dimerizing fluids from "experimental" diffraction data by reverse Monte Carlo modelling', *Revista Mexicana de Física* **49**, 212-218 (2003) IF: 0.20

61) S. Kugler, K. Kohary, K. Kádas, L. Pusztai, 'Small bond angles in amorphous silicon: are they a new type of defect?', *J. Non-Cvryst. Sol.*, **338-340**, 425-429 (2004) IF: 1.43

62) L. Temleitner, Gy. Mészáros, L. Pusztai, E. Sváb, 'Neutron diffraction studies of molecular liquids using the new detector system of the PSD diffractometer at the Budapest Research Reactor', *Physica B*, **350**, E865-E867 (2004) IF: 0.68

63) L. Pusztai, H. Dominguez, O.A. Pizio, ' Reverse Monte Carlo Modelling of the Structure of Colloidal Aggregates', *J. Coll. Int. Sci*., **227**, 327-334 (2004 May) IF: 1.78

SUM2003_2004=11.42

64) L. Temleitner, L. Pusztai, 'Orientational correlations in liquid carbon monoxide and nitric oxide', *J. Phys.: Cond. Matter* **17**, S47-S57 (2005 January) IF: 2.15

65) I. Harsányi, L. Pusztai, 'On the structure of aqueous hydrogen-chloride solutions', *J. Phys.: Cond. Matter* **17**, S59-S65 (2005 January) IF: 2.15

66) G. Evrard, L. Pusztai, 'Data vs. constraints in RMC modelling: case study with molecular liquid CCl_4', *J. Phys.: Cond. Matter* **17**, S37-S46 (2005 January) IF: 2.15

67) G. Evrard, L. Pusztai, 'Reverse Monte Carlo modelling of the structure of disordered materials with RMC++: a new implementation of the algorithm in C++', *J. Phys.: Cond. Matter* **17**, S1-S13 (2005 January) https://doi.org/10.1088/0953-8984/17/5/001 IF: 2.15

68) I. Harsányi, L. Pusztai, 'On the structure of aqueous lithium-chloride solutions', *J. Chem. Phys* **122,** 124512 (2005 April) https://doi.org/10.1063/1.1877192 IF: 3.14

69) L. Pusztai, S. Kugler, 'Comparison of the structures of evaporated and ion-implanted amorphous silicon samples', *J. Phys.: Cond Matter* **17,** 2617-2624 (2005 April) IF: 2.15
SUM2005=13.89

70) L. Pusztai, R.L. McGreevy, 'On the structure of simple liquids $SbCl_5$ and WCl_6', *J. Chem. Phys* **125,** 044508/1-7 (2006 July) IF: 3.14

71) I. Harsányi, L. Pusztai, J.-C. Soetens, L. Pusztai, 'Molecular dynamics simulations of aqueous RbBr solutions over the entire solubility range', *J. Mol. Liq*., **129**, pp. 80-85 (2006 November) https://doi.org/10.1016/j.molliq.2006.08.005 IF: 0.83

72) P. Jóvári, L. Pusztai, 'Structural changes in liquid selenium with increasing temperature', *J. Mol. Liq*., **129**, pp. 115-119 (2006 November) IF: 0.83
SUM2006=4.8

73) I. Harsányi, P. Jóvári, Gy. Mészáros, L. Pusztai, Ph. A. Bopp, 'Neutron and X-ray diffraction studies of aqueous rubidium bromide solutions', *J. Mol. Liq.*,**131-132**, pp. 60-64 (2007 March) IF: 0.83

74) T. Arai, L. Pusztai, R.L. McGreevy, 'Polyanions in molten KPb—a paradox explained?', *J. Phys.: Condens. Matter* **19**, 335202 (10pp) (2007 August) IF: 2.15

75) L. Temleitner, L. Pusztai, 'Orientational correlations in liquid, supercritical and gaseous carbon dioxide', *J. Phys.: Condens. Matter* **19**, 335203 (12pp) (2007 August) IF: 2.15

76) Sz. Pothoczki, L. Pusztai, S. Kohara, 'The structure of liquid iodomethane, CH_3I/CD_3I', *J. Phys.: Condens. Matter* **19**, 335204 (9pp) (2007 August) IF: 2.15

77) B. Gabrys, L. Pusztai, D.G. Pettifor, 'On the structure of liquid phosphorous tribromide (PBr_3)', *J. Phys.: Condens. Matter* **19**, 335205 (10pp) (2007 August) IF: 2.15

78) L. Temleitner, L. Pusztai, W. Schweika, 'The structure of liquid water by polarized neutron diffraction and reverse Monte Carlo modelling', *J. Phys.: Condens. Matter* **19**, 335207 (12pp) (2007 August) IF: 2.15

79) I. Harsányi, L. Pusztai, 'Hydration of ions in aqueous RbCl solutions', *J. Phys.: Condens. Matter* **19**, 335208 (12pp) (2007 August) IF: 2.15

80) O. Gereben, L. Pusztai, R.L. McGreevy, 'Development of the time-dependent reverse Monte Carlo simulation, RMC*t*', *J. Phys.: Condens. Matter* **19**, 335223 (22pp) (2007 August) IF: 2.15

81) O. Gereben, P. Jóvári, L. Temleitner, L. Pusztai, 'A new version of the RMC++ Reverse Monte Carlo programme, aimed at investigating the structure of covalent glasses', *J. Optoel. Adv. Mater*. **9**, pp. 3021-3027 (2007 October) https://old.joam.inoe.ro/index.php?option=magazine&op=view&idu=953&catid=18 IF: 1.11

82) H. Dominguez, O. Pizio, L. Pusztai, S. Sokolowski, 'The Structural Properties and

Diffusion of a Three-dimensional Isotropic Core-softened Model Fluid in Disordered Porous Media. Molecular Dynamics Simulation', *Adsorption Science&Technology* **25**, pp.479-491 (2007) IF: 0.56

SUM2007=17.55

83) L. Pusztai, I. Harsányi, H. Dominguez, O. Pizio, 'Assessing the level of consistency between diffraction experiments and interaction potentials: A combined molecular dynamics (MD) and Reverse Monte Carlo (RMC) approach', *Chem. Phys. Letts*. **457**, pp. 96-102 (2008 April) https://doi.org/10.1016/j.cplett.2008.03.091 IF: 2.17

84) L. Temleitner, L. Pusztai, Y. Akahama, H. Kawamura, S. Kohara, Y. Ohishi, M. Takata, 'Orientational correlations in high-pressure fluid oxygen and nitrogen', *Phys. Rev. B* **78**, 014205/1-6 (2008July) IF: 3.32

85) L. Pusztai, Sz. Pothoczki, S. Kohara, 'Orientational correlations in molecular liquid SnI_4', *J. Chem. Phys*. **129**, 064509/1-4 (2008) IF: 3.15

86) L. Pusztai, O. Pizio, S. Sokolowski, 'Comparison of interaction potentials of liquid water with respect to their consistency with neutron diffraction data of pure heavy water', *J. Chem. Phys*., **129** 184103 (2008) https://doi.org/10.1063/1.2976578 IF: 3.15

SUM2008=11.79; SUM1987-2008=152,18

87) Sz. Pothoczki, L. Temleitner, P. Jóvári, S. Kohara, L. Pusztai, 'Nanometer range correlations between molecular orientations in liquids of molecules with perfect tetrahedral shape: CCl_4, $SiCl_4$, $GeCl_4$ and $SnCl_4$', *J. Chem. Phys*., **130** 064503 (2009) IF: 3.093

88) Sz. Pothoczki, L. Pusztai, 'Molecular liquid $TiCl_4$ and VCl_4: Two substances, one structure ?', *J. Mol. Liq*.**145**, pp. 38-40 (2009) IF: 1.278

89) R. Vácha, T. Megyes, I. Bakó, L. Pusztai, P. Jungwirth, 'Benchmarking polarizable molecular dynamics simulations of aqueous sodium hydroxide by diffraction measurements', *Journal of Physical Chemistry A*, **113** 4022-4027 (2009) IF: 2.87

90) L. Pusztai, H. Dominguez, O. Pizio, S. Sokolowski, 'Detailed structural analysis of a 2 molal aqueous rubidium bromide solution : A combined molecular dynamics and Reverse Monte Carlo approach', *J. Mol. Liq*., **147**, pp. 52-55 (2009) IF: 1.278

91) K. Ohara, Y. Kawakita, L. Temleitner, L. Pusztai, S. Kohara, A. Jono, H. Shimakura, N. Inoue, S. Takeda, 'Structural analysis of Lithium Lanthanum Titanate with perovskite structure', *Physica Status Solidi: C*., **6**, 1004-1007 (2009) IF: approx. 1.0

92) O. Pizio, L. Pusztai, Z. Sokolowska, S. Sokolowski, 'Solvation force between surfaces modified by tethered chains: a density functional approach', *J. Chem. Phys*., **130**,

13401/1-10 (2009) IF: 3.093

93) Viktória Mile, László Pusztai, Hector Dominguez, and Orest Pizio, 'Understanding the Structure of Aqueous Cesium Chloride Solutions by Combining Diffraction Experiments, Molecular Dynamics Simulations, and Reverse Monte Carlo Modeling', *J. Phys. Chem B*, **113**, 10760-10769 (2009) https://doi.org/10.1021/jp900092g IF: 3.471

94) O. Pizio, H. Dominguez, L. Pusztai, S. Sokolowski, 'A core-softened model fluid in disordered porous media. Grand-canonical Monte Carlo simulation and integral equations', *Physica A* **388**, 2278-2288 (2009) IF: 1.562

SUM2009=17.645

95) Ohara K, Kawakita Y, Pusztai L, Temleitner L, Kohara S, Inoue N, Takeda S; Lattice Distortion and Lithium Conduction Path in a Superionic Conductor with Perovskite Structure; *J. Phys. Soc. Jpn;*. **79** Suppl. A, pp. 94-97, (2010) IF: 2.905

96) Sz. Pothoczki, S. Kohara, L. Pusztai, 'Partial radial distribution functions of methylene halide molecular liquids', *J. Mol. Liq.* **153**, 112-116 (2010) IF: 1.649

97) Sz. Pothoczki, L. Temleitner, L. Pusztai, 'Extended orientational correlation study for molecular liquids containing distorted tetrahedral molecules: Application to methylene halides', *J. Chem. Phys.* **132**, 164511/1-7 (2010). IF: 2.92

98) L. Temleitner, L. Pusztai, 'Local order and orientational correlations in liquid and crystalline phases of carbon tetrabromide from neutron powder diffraction measurements', *Phys. Rev. B* **81**, 134101/1-8 (2010). IF: 3.475

99) O. Gereben, L. Pusztai, R.L. McGreevy, 'RMCSANS - modelling the inter-particle term of small angle scattering data via the reverse Monte Carlo method', *J. Phys: Condens. Matter* **22,** 404216/1-12 (2010) IF: 1.964

100) Sz. Pothoczki, L. Temleitner, S. Kohara, P. Jóvári, L. Pusztai, 'The liquid structure of haloforms $CHCl_3$ and $CHBr_3$', *J. Phys: Condens. Matter* **22**, 404211/1-9 (2010) IF: 1.964

101) A. Vrhovsek, O. Gereben, Sz. Pothoczki, M. Tomsic, A. Jamnik, S. Kohara, L. Pusztai, 'The approach towards understanding the structure of complex molecular systems: the case of lower aliphatic alcohols', *J. Phys: Condens. Matter* **22,** 404214/1-9 (2010) IF: 1.964

102) K. Ohara, Y. Kawakita, L. Pusztai, L. Temleitner, S. Kohara, N. Inoue, S. Takeda, 'Structural disorder in lithium lanthanum titanate: the basis of superionic conduction', *J. Phys: Condens. Matter* **22,** 404203/1-9 (2010) IF: 1.964

103) V. Mile, O. Gereben, S. Kohara, L. Pusztai, 'On the structure of aqueous cesium bromide solutions: diffraction experiments, molecular dynamics simulations and Reverse Monte Carlo modeling', *J. Mol. Liq.* **157,** pp. 36-42 (2010)

https://doi.org/10.1016/j.molliq.2010.08.003 IF: 1.649

104) Kohara S, Ohno H, Takata M, Usuki T, Morita M, Suzuya K, Akola J, Pusztai L; Lead silicate glasses: binary network-former glasses with unusually large amounts of free volume; *Phys. Rev. B*; **82**, 134209/1-7 (2010) IF: 3.475

SUM2010: 23.929

105) Harsányi I, Bopp PA, Vrhovšek A, Pusztai L; On the hydration structure of LiCl aqueous solutions: a Reverse Monte Carlo based combination of diffraction data and Molecular Dynamics simulations; *J. Mol. Liq.* **158**, pp. 61-67 (2011) https://doi.org/10.1016/j.molliq.2010.10.010 IF: 1.58

106) Pothoczki Sz, Temleitner L, Pusztai L; Detailed intermolecular structure of molecular liquids containing slightly distorted tetrahedral molecules with C_{3v} symmetry: chloroform, bromoform and methyl-iodide; *J. Chem. Phys*. **134**, 044521/1-8 (2011); IF: 3.33

107) Gereben O, Pusztai L; On the accurate calculation of the dielectric constant from molecular dynamics simulations: the case of SPC/E and SWM4-DP water; *Chem. Phys. Lett*s. **507**, pp. 80-83 (2011) https://doi.org/10.1016/j.cplett.2011.02.064 IF: 2.37

108) Gereben O, Pusztai L; System size and trajectory length dependence of the static structure factor and the diffusion coefficient as calculated from molecular dynamics simulations: the case of SPC/E water; *J. Mol. Liq.*, **161**, pp. 36-40 (2011) https://doi.org/10.1016/j.molliq.2011.04.004 IF: 1.58

109) Gereben O, Pusztai L; Extension of the invariant environment refinement technique + reverse Monte Carlo method of structural modelling for interpreting experimental structure factors: The cases of amorphous silicon, phosphorus, and liquid argon; *J. Chem. Phys.,* **125,** 084111/1-6 (2011). IF: 3.33

110) Vrhovšek A, Gereben O, Jamnik A, Pusztai L; Hydrogen Bonding and Molecular Aggregates in Liquid Methanol, Ethanol and Propanol; *J. Phys. Chem B*; **115**, 13473-13488 (2011). https://doi.org/10.1021/jp206665w IF: 3.70

SUM-2011=15.89

111) Harsányi I, Temleitner L, Beuneu B, Pusztai L; Neutron and X-ray diffraction measurements on highly concentrated aqueous LiCl solutions; J. Mol. Liq. **165**, 94-100 (2012) IF: 1.58

112) Ohara K, Temleitner L, Sugimoto K, Kohara S, Matsunaga T, Pusztai L, Itou M, Ohsumi H, Kojima R, Yamada N, Usuki T, Fujiwara A, Takata M; The roles of the Ge-Te core network and the Sb-Te pseudo network during rapid nucleation-dominated crystallization of amorphous $Ge_2Sb_2Te_5$; Advanced Functional Materials; **22**, 2251-2257, DOI: 10.1002/adfm.201102940 (2012) IF: 9.79

113) Gereben O, Kohara S, Pusztai L; The liquid structure of some food aromas: joint

X-ray diffraction, all-atom Molecular Dynamics and Reverse Monte Carlo investigations of dimethyl sulfide, dimethyl disulfide and dimethyl trisulfide; Journal of Molecular Liquids; **169**, 63-73 (2012); IF: 1.58

114) Antipas GSE, Temleitner L, Karalis K, Kohara S, Pusztai L, Xenidis A; A containerless study of short-range order in high-temperature Fe-Si-Al-Ca-Mg-Cr-Cu-Ni oxide systems; Journal of Molecular Structure **1019**, 151-158 (2012); IF: 1.63

115) Steinczinger Zs, Pusztai L; An independent, general method for checking consistency between diffraction data and partial radial distribution functions derived from them: the example of liquid water; Condensed Matter Physics **15**, 23606:1-6 (2012); IF: 0.81

116) Gereben O, Pusztai L; Molecular Conformations and the Liquid Structure in Bis(methylthio)methane and Diethyl Sulfide: Diffraction Experiments vs Molecular Dynamics Simulations; J. Phys. Chem. B, 116, pp. 9114-9121 (2012); IF: 3.70

117) Mile V, Gereben O, Kohara S, Pusztai L; On the Structure of Aqueous Cesium Fluoride and Cesium Iodide Solutions: Diffraction Experiments, Molecular Dynamics Simulations and Reverse Monte Carlo Modeling; J. Phys. Chem. B, 116, pp. 9758-9767 (2012); IF: 3.70

118) Gereben O, Pusztai L; RMC_POT, a computer code for Reverse Monte Carlo modeling the structure of disordered systems containing molecules of arbitrary complexity; Journal of Computational Chemistry; Volume 33, Issue 29, 5 November 2012, Pages: 2285–2291 (2012); doi: 10.1002/jcc.23058 IF: 4.58

119) Temleitner L, Pusztai L, Rubio-Arroyo MF, Aguilar-Lopez S, Klimova T, Pizio O; Microscopic and mesoscopic structural features of an activated carbon sample, prepared from sorghum via activation by phosphoric acid; Materials Research Bulletin, 47, pp. 4409-4413 (2012); IF: 2.1

120) Harsányi I, Pusztai L; Hydration structure in concentrated aqueous lithium chloride solutions: A reverse Monte Carlo based combination of molecular dynamics simulations and diffraction data; J. Chem. Phys. 137, 204503/1-9 (2012) IF: 3.33

SUM-2012=32.8

121) Gereben O; Pusztai L; Conformational analyses of bis(methylthio)methane and diethyl sulfide molecules in the liquid phase: reverse Monte Carlo studies using classical interatomic potential functions; J. Phys.: Condensed Matter 25, 454201 (2013) IF: 2.36

122) Antipas G; Temleitner L; Karalis K; Pusztai L; Xenidis A; Atomic order and cluster energetics of a 17 w.t.% Si-based glass versus the liquid phase; J. Phys.: Condensed Matter 25, 454206 (2013) IF: 2.36

123) Temleitner L; Pusztai L; The origin of diffuse scattering in crystalline carbon tetraiodide; J. Phys.: Condensed Matter 25, 454209 (2013) IF: 2.36

124) Harsányi I; Pusztai L; Jovari P; Beuneu B; Acidic properties of aqueous phosphoric acid solutions: a microscopic view; J. Phys.: Condensed Matter 25, 454215 (2013) IF: 2.36

125) Shimakura H; Kawakita Y; Ohara K; Pusztai L; Wakisaka Y; Takeda S; Intermolecular correlations in liquid Se_2Br_2; J. Phys.: Condensed Matter 25, 454221 (2013) IF: 2.36

126) Gereben O; Pusztai L; The liquid structure of tetrachloroethene: molecular dynamics simulations and Reverse Monte Carlo modeling with interatomic potentials; J. Chem. Phys., **139**, 164509 (2013) IF: 3.16

127) Steinczinger Zs; Pusztai L; Comparison of the TIP4P-2005, SWM4-DP and BK3 interaction potentials of liquid water with respect to their consistency with neutron and X-ray diffraction data of pure water; Condensed Matter Physics; vol. **16**, No. 4, 43604:1-8 (2013)
IF: 0.76

SUM.2013= 15.72

128) Karalis K , Temleitner L , Antipas GSE , Pusztai L , Xenidis A; Experimentally constrained atomic order probing of a Si-Al composite glass; ***PHILOSOPHICAL MAGAZINE*** 94:(8) pp. 792-800. (2014) IF:1.43

129) Kohara S , Tajiri H , Song CH , Ohara K , Temleitner L , Sugimito K , Fujiwara A , Pusztai L , Usuki T , Hosokawa S , Benino Y , Kitamura N , Fukumi K; Anomalous x-ray scattering studies of functional disordered materials; ***JOURNAL OF PHYSICS-CONFERENCE SERIES*** 502:(1) Paper 012014. 6 p. (2014) IF:1.0 (???)

130) Pothoczki S , Temleitner L , Pusztai L; The structure of PX_3 (X = Cl, Br, I) molecular liquids from X-ray diffraction, molecular dynamics simulations, and reverse Monte Carlo modeling; ***JOURNAL OF CHEMICAL PHYSICS*** 140:(5) Paper 054504. 9 p. (2014) IF:3.12

SUM-2014=4.55

131) Gereben O, Pusztai L; Understanding the structure of molecular liquids via combinations of molecular dynamics simulations and Reverse Monte Carlo modeling: Handling information deficiency; *Journal of Non-Crystalline Solids* **407,** pp. 213–219 (2015) IF: 1.72

132) Gereben O, Pusztai L; Investigation of the Structure of Ethanol/Water Mixtures by Molecular Dynamics Simulation I: Analyses Concerning the Hydrogen-Bonded Pairs; *Journal of Physical Chemistry B*; **119**, pp 3070–3084 (2015); DOI: 10.1021/jp510490y IF: 3.38

133) Sanchez V, Noya EG, Temleitner L, Pusztai L; Reverse Monte Carlo modeling: the two distinct routes of calculating the experimental structure factor; *Journal of Molecular Liquids*; **207**, pp. 211-215 (2015) IF: 2.74

134) Galicia-Andres E, Pusztai L, Temleitner L, Pizio O; Microscopic structure of methanol–water mixtures: Synchrotron X-ray diffraction experiments and molecular dynamics simulations over the entire composition range; *Journal of Molecular Liquids*; **209**, pp. 586-595 (2015) DOI:10.1016/j.molliq.2015.06.045 IF: 2.74

135) Temleitner L, Stunault A, Cuello G, Pusztai L; Neutron diffraction of hydrogenous materials: Measuring incoherent and coherent intensities separately; *Phys. Rev. B* **92**, 014201/1-6 (2015) IF: 3.7

136) Galicia-Andres E, Dominguez H, Pusztai L, Pizio O; Composition dependence of thermodynamic, dynamic and dielectric properties of water–methanol model mixtures. Molecular dynamics simulation results with the OPLS-AA model for methanol; *J. Mol. Liq.* Volume **212**, Pages 111-116 (2015) 10.1016/j.molliq.2015.08.061. IF: 2.74

137) Pethes I, Pusztai L; Reverse Monte Carlo investigations concerning recent isotopic substitution neutron diffraction data on liquid water; J. Mol. Liq. Volume 212, Pages 70-78 (2015) IF: 2.74

138) Galicia-Andres E, Dominguez H, Pusztai L, Pizio O; On the composition dependence of thermodynamic, dynamic and dielectric properties of water-methanol model mixtures. Molecular dynamics simulation results; *Condensed Matter Physics*, vol. **18**, No. 4, p. 43602 (2015) IF: 0.76

139) Pothoczki Sz, Temleitner L, Pusztai L; Structure of Neat Liquids Consisting of (Perfect and Nearly) Tetrahedral Molecules; *Chemical Reviews*; **115**, No. 24, pp 13308–13361 (2015), DOI: 10.1021/acs.chemrev.5b00308 IF: 37.37. D1

140) Rodriguez Palomino LA; Stunault A; Dawidowski J; Temleitner L, Pusztai L; Cuello GJ; A Monte Carlo simulation code applied to dffraction experiments with polarization analysis; *J. Phys.: Conference Series* **663,** 012002/1-10 (2015); doi:10.1088/1742-6596/663/1/012002 IF: ca. 1.0 (????)

SUM-2015=57.89

SUM-1988-2015= 320.604

141) Sánchez-Gil V; Noya E; Guil J; Lomba E; Valencia S; Da Silva I; Pusztai L; Temleitner L; Evidences of a Structural Change in Pure-Silica MEL upon the Adsorption of Argon; *J. Phys. Chem. C*, **120**, pp. 2260-2270. (2016) IF: 4.77 D1

142) Tscheliessnig R; Pusztai L; Proteins in solution: fractal surfaces in solutions; *Condensed Matter Physics (Lviv)*, Vol. 19, No 1, 13803: 1–8 DOI: 10.5488/CMP.19.13803 IF: 0.76 Q3

143) Méndez-Bermudez JG; Dominguez H; **Pusztai L**, Guba S; Horváth B; Szalai I; Composition and temperature dependence of the dielectric constant of 1-propanol/water mixtures: experiment and molecular dynamics simulations*; J. Mol. Liq.*, 219, pp. 354–358 (2016) DOI: 10.1016/j.molliq.2016.02.053 IF: 3.648 Q1

144) Stunault A; Vial S; **Pusztai L**; Cuello GJ; Temleitner L; Structure of hydrogenous liquids: separation of coherent and incoherent cross sections using polarised neutrons; *J. Phys.: Conference Series* **711** 012003 /1-5 (2016); doi:10.1088/1742-6596/711/1/012003 IF: cca. 1.0 (?????) Q3

145) Gereben O; **Pusztai L**; Hydrogen bond connectivities in water–ethanol mixtures: On the influence of the H-bond definition; *J. Mol. Liq.*, **220**, pp. 836–841 (2016) DOI: http://dx.doi.org/10.1016/j.molliq.2016.05.035 IF: 3.648 Q1

SUM-2016= 12.826

146) Pothoczki Sz; **Pusztai L**; Intermolecular orientations in liquid acetonitrile: New insights based on diffraction measurements and all-atom simulations; *Journal of Molecular Liquids*; **225**, Pages 160-166, (2017); DOI: http://dx.doi.org/10.1016/j.molliq.2016.11.056 IF: 3.648 Q1

147) Steinczinger Zs; Jóvári P; **Pusztai L**; Comparison of interatomic potentials of water via structure factors reconstructed from simulated partial radial distribution functions: a reverse Monte Carlo based approach; *Physica Scripta*; **92,** 014001 (7pp) (2017); doi:10.1088/0031-8949/92/1/014001 IF: 1.2 Q3

148) Steinczinger Zs; Jóvári P; **Pusztai L**; Comparison of 9 classical interaction potentials of liquid water: simultaneous Reverse Monte Carlo modeling of X-ray and neutron diffraction results and partial radial distribution functions from computer simulations; *J. Mol. Liq.*, **228**, pp. 19-24 (2017) DOI: http://dx.doi.org/10.1016/j.molliq.2016.09.068 IF: 3.648 Q1

149) Gujt J; Cázares Vargas E; **Pusztai L**; Pizio O; On the composition dependence of thermodynamic, dynamic and dielectric properties of water-dimethyl sulfoxide model mixtures. NPT molecular dynamics simulation results; *J. Mol. Liq.*, **228**, pp. 71-80 (2017); DOI: http://dx.doi.org/10.1016/j.molliq.2016.09.024 IF: 3.648 Q1

150) Bakó I; Oláh J; Lábas A; Bálint Sz; **Pusztai L**; Bellissent-Funel M-C;

Water-formamide mixtures: Topology of the hydrogen-bonded network; *J. Mol. Liq*., **228**, pp. 25-31 (2017); DOI: http://dx.doi.org/10.1016/j.molliq.2016.10.052 IF: 3.648 Q1

151) Pethes I; **Pusztai L**; Reverse Monte Carlo modeling of liquid water with the explicit use of the SPC/E interatomic potential; *J. Chem. Phys*., **146**, 064506 (2017); DOI: 10.1063/1.4975987 IF: 2.89 Q1

152) Bakó I; **Pusztai L**; Temleitner L; Decreasing temperature enhances the formation of sixfold hydrogen bonded rings in water-rich water-methanol mixtures; *Scientific Reports*; 7, Art. No. 1073 (7 pp) (2017); DOI: doi:10.1038/s41598-017-01095-7 IF: 4.2 D1

153) Gereben O; **Pusztai L**; Cluster formation and percolation in ethanol-water mixtures; *Chem. Phys*.; **496,** 1-8 (2017); DOI: http://dx.doi.org/10.1016/j.chemphys.2017.09.003 IF: 2.05 Q2

SUM_2017= 24.93

154) Pothoczki Sz; **Pusztai L**; Bakó I; Variations of the Hydrogen Bonding and Hydrogen-Bonded Network in Ethanol−Water Mixtures on Cooling; *J. Phys Chem. B*; **122**, 6790−6800 (2018); DOI: 10.1021/acs.jpcb.8b02493 IF: 3.15 D1

155) Pothoczki Sz; **Pusztai L**; Bakó I; Temperature dependent dynamics in water-ethanol liquid mixtures; *J. Mol. Liq*.; **271,** 571–579 (2018); DOI: https://doi.org/10.1016/j.molliq.2018.09.027 IF: 4.5 Q1

156) Pethes I; Temleitner L; Tomsic M; Jamnik A; **Pusztai L**; Unexpected Composition Dependence of the First Sharp Diffraction Peak in an Alcohol–Aldehyde Liquid Mixture: n-Pentanol and Pentanal; *phys. stat. sol (b)*; **255**, 1800130/1-7 (2018); DOI: 10.1002/pssb.201800130 IF: 1.72 Q2

157) Pethes I; Temleitner L; Tomsic M; Jamnik A; **Pusztai L**; X-Ray Diffraction and Computer Simulation Studies of the Structure of Liquid Aliphatic Aldehydes: From Propanal to Nonanal; *phys. stat. sol (b)*; **255**, 1800127/1-7 (2018); DOI: 10.1002/pssb.201800127 IF: 1.72 Q2

158) Mendez-Bermudez JG; Dominguez H; Temleitner L; **Pusztai L**; On the Structure Factors of Aqueous Mixtures of 1-Propanol and 2-Propanol: X-Ray Diffraction Experiments and Molecular Dynamics Simulations; *phys. stat. sol (b);* **255**, 1800215/1-8 (2018); DOI: 10.1002/pssb.201800215 IF: 1.72 Q2

SUM_2018= 12.81

159) Bakó I; Pethes I; Pothoczki Sz; **Pusztai L**; Temperature dependent

network stability in simple alcohols and pure water: The evolution of Laplace spectra; *J. Mol Liq.*; **273**, 670-675 (2019); DOI: https://doi.org/10.1016/j.molliq.2018.11.021 IF: 4.5 Q1

160) Bakó I; Mayer I; Hamza A; **Pusztai L**; Two- and three-body, and relaxation energy terms in water clusters: Application of the hierarchical BSSE corrected decomposition scheme; *Journal of Molecular Liquids*, **285**, 171-177 (2019). DOI: https://doi.org/10.1016/j.molliq.2019.04.088; IF: 4.5 Q1

161) Pothoczki, Sz; **Pusztai, L**; Bakó, I; Molecular Dynamics Simulation Studies of the Temperature Dependent Structure and Dynamics of Isopropanol-Water Liquid Mixtures at Low Alcohol Content; *J. Phys Chem. B*; **123,** 7599-7610 (2019); DOI: 10.1021/acs.jpcb.9b05631 IF: 2.93 Q1

162) Hosokawa, S; Bérar, J-F; Boudet, N; Pilgrim, **Pusztai, L**; Hiroi, S; Maruyama, K; Kohara, S; Kato, H; Fischer, HE; Zeidler, A; Partial structure investigation of the traditional bulk metallic glass Pd40Ni40P20; *Phys. Rev. B*; **100**, 054204 (2019); DOI: https://doi.org/10.1103/PhysRevB.100.054204; IF: 3.74 D1

163) Bakó, I; Daru, J; Pothoczki, Sz; **Pusztai, L**; Hermansson, K; Effects of H-bond asymmetry on the electronic properties of liquid water – an AIMD analysis; *Journal of Molecular Liquids*, **293,** 111579; (2019); DOI: https://doi.org/10.1016/j.molliq.2019.111579 IF: 4.5 Q1

SUM_2019: 20.17

164) Cerar, J; Jamnik, A; Pethes, I; Temleitner, L; **Pusztai, L**; Tomšič, M; Structural, rheological and dynamic aspects of hydrogen-bonding molecular liquids: Aqueous solutions of hydrotropic *tert*-butyl alcohol; *J. Coll. Interf. Sci*., **560**, pp. 730-742 (2020); DOI: https://doi.org/10.1016/j.jcis.2019.10.094. IF: 7.489 Q1 (D1 in some areas)

165) Pethes, I; Bakó, I; **Pusztai, L**; Chloride ions as integral parts of hydrogen bonded networks in aqueous salt solutions: the appearance of solvent separated anion pairs; *Physical Chemistry Chemical Physics (PCCP)*, **22**, pp. 11038-11044. (2020) DOI: https://doi.org/10.1039/D0CP01806F IF: 3.43 Q1

166) Pethes, I; **Pusztai, L**; Ohara, K; Kohara, S; Darpentigny, J; Temleitner, L; Temperature-dependent structure of methanol-water mixtures on cooling: X-ray and neutron diffraction and molecular dynamics simulations; *Journal of Molecular Liquids,* **314**, Paper: 113664, 10 p. (2020) DOI: https://doi.org/10.1016/j.molliq.2020.113664 IF: 5.065 Q1

SUM_2020: 15.98

SUM_1987-2020: 407.354

167) Hosokawa, S; Bérar, J-F; Boudet, N; Pilgrim, W-C; **Pusztai, L**; Hiroi, S; Kohara, S; Kato, H; Fischer, HE; Zeidler, A; Detailed structural analysis of amorphous $Pd_{40}Cu_{40}P_{20}$: Comparison with the metallic glass $Pd_{40}Ni_{40}P_{20}$ from the viewpoint of glass forming ability; *J.Non-Cryst. Solids*, **552** Paper: 120536 , 10 p. (2021) IF: 2.99 Q1

168) Bakó, I.; Madarász, Á.; **Pusztai, L**. Nuclear quantum effects: Their relevance in neutron diffraction studies of liquid water. *J. Mol. Liq*. **325** Paper: 115192 , 8 p. (2021) IF: 5.065 Q1

169) Hosokawa, S; Kawakita, Y; **Pusztai, L**; Ikeda, K; Otomo, T; Detailed investigations on short- and intermediate-range structures of Ge-Se glasses near the stiffness transition composition; *J. Phys. Soc. Jpn*., **90** 024601, 12 p. (2021) IF: 1.58 Q2

170) Pothoczki, Sz; Pethes, I; **Pusztai, L**; Temleitner, L; Csókás, D; Kohara, S; Ohara, K; Bakó, I; Hydrogen bonding and percolation in propan-2-ol – Water liquid mixtures: X-ray diffraction experiments and computer simulations; *J. Mol. Liq*. **329** Paper:115592, 10 p. (2021) IF: 5.065 Q1

171) Temleitner, L.; Hattori, T; Abe, J; Nakajima, Y; **Pusztai, L**; Pressure-Dependent Structure of Methanol–Water Mixtures up to 1.2 GPa: Neutron Diffraction Experiments and Molecular Dynamics Simulations; *Molecules* **26(5)**, 1218, 13 p. (2021); https://doi.org/10.3390/molecules26051218 IF: 3.267 Q2(/Q1)

172) Hosokawa, S; Kawakita, Y; Stellhorn, JR; **Pusztai, L**; Blanc, N; Boudet, N; Ikeda, K; Otomo, T; Local- and Intermediate-Range Atomic Structures on Room-Temperature Superionic-Conducting Ag-GeSe3 Glasses; *J. Phys. Soc. Jpn. -- Conf. Proceedings (JPS Conf. Proc.), 3rd J-PARC Symposium (J-PARC2019)*, **33,** 011070 (2021) https://doi.org/10.7566/JPSCP.33.011070 IF: --none--

173) Hosokawa, S; Stellhorn, JR; Onodera, Y; Kohara, S; Magome, E; **Pusztai, L**; Ikeda, K; Otomo, T; Krbal, M; Wagner, T; Local- and Intermediate-Range Atomic Order in Ga2Ge3Se9 Glass: Complementary Use of X-Rays and Neutrons; ; *J. Phys. Soc. Jpn. -- Conf. Proceedings (JPS Conf. Proc.), 3rd J-PARC Symposium (J-PARC2019)*, **33**, 011069 (2021) https://doi.org/10.7566/JPSCP.33.011069 IF: --none—

174) Pothoczki, S; Pethes, I; **Pusztai, L**; Temleitner, L; Ohara, K; Bakó, I; Properties of Hydrogen-Bonded Networks in Ethanol–Water Liquid Mixtures as a Function of Temperature: Diffraction Experiments and Computer Simulations; The Journal of Physical Chemistry B; Article ASAP (2021); DOI:

10.1021/acs.jpcb.1c03122. IF: 2.857

175) Bakó, I; Csókás, D; Mayer, I; Pothoczki, S; **Pusztai, L**; The influence of cations on the dipole moments of neighboring polar molecules; Int J. Quant. Chem., accepted (2021) IF: 1.747

SUMMA IF (2016-2020): ca. 87.82

SUMMA IF: 434.06 (up to #171 + 1-13below)

Books, book chapters, review articles

i) In Hungarian:

1) Baranyai András, Pusztai László, 'Disorder in Condensed Phases' (*Latest Developments in Chemistry*, **Vol**. **80**, Akadémiai Kiadó, Budapest, 1995.) (in Hungarian)

2) Pusztai L., 'The Reverse Monte Carlo Simulation: Preliminaries, Technical Details, Results', *Kém. Közl.* **75**, pp. 185-258 (1992) (in Hungarian)

ii) In English:

3) L Pusztai, `On the Atomic Structure of Amorphous Semiconductors', *Solid State Phenomena* **44-46**, 25 (1995)

4) L Pusztai, `Reverse Monte Carlo simulations for determining disordered structures. Basics, and application for amorphous semiconductors', *NATO ASI Series Volume 3/23. `Amorphous insulators and semiconductors', Eds.:M.F. Thorpe and M. Mitkova, (Kluwer Academic Publishers)*, pp. 215-224 (1997)

5) P. Jóvári, L. Pusztai, 'Structural changes across phase transitions in disordered systems: Liquid sulphur, liquid phosphorus and amorphous ice', *NATO ARW Series 'New kinds of phase transitions: Transformations in disordered substances', Eds.: V. V. Brazhkin, S. Buldyrev, H.E. Stanley and V. Ryzhov (Kluwer Academic Publishers),* pp. 267-282 (2002)

6) L. Pusztai, 'Neutron scattering methods in Chemistry', Handbook of Nuclear Chemistry, Eds. A. Vértes, S. Nagy, Z. Klencsár, Vol. **3**, Chapter 7, pp. 1-41 (2003)

7) Pusztai L; 'Reverse Monte Carlo modelling of diffraction data: structural studies of amorphous ices'; Erice Course on *High Pressure Crystallography; Eds. A. Katrusiak and P.F. McMillan, NATO Science Series II*. (Kluwer Academic Publishers, Doordrect, The Netherlands); Vol. **140**; pp. 237-256 (2004)

8) Pusztai L*; '*Reverse Monte Carlo analyses of diffraction data on molecular liquids'; *Novel Approaches to the Structure and Dynamics of Liquids;* Eds. J. Samios, V.A. Durov, NATO Science Series II. (Kluwer Academic Publishers, Doordrect, The Netherlands); Vol. **133**; pp.129-142 (2004)

9) L. Temleitner, L. Pusztai; 'Investigation of the structural disorder in ice Ih using neutron diffraction and Reverse Monte Carlo modelling'; Physics and Chemistry of Ice; Ed. W. F. Kuhs (Royal Society of Chemistry Publishing, Cambridge, UK); pp. 593-600 (2007)

10) Pothoczki Sz, Temleitner L, Pusztai L; Determination of molecular orientational correlations in disordered systems from diffraction data; *Advances in Chemical Physics*; **150**, pp. 143-168 (2012) IF: 3.58

Conference Abstracts (referred and cited by ISI)

1) L. Pusztai; 'Reverse Monte Carlo modelling of amorphous alloys and covalent glasses'*; Acta Cryst*. **A58** (Supplement), C48 (2002) IF: 1.72
2) L. Temleitner, L. Pusztai: Orientational ordering in liquids of diatomic molecules, *Acta Cryst.* **A 60** (Supplement), S259 (2004) IF: 1.72
3) I. Harsányi, L. Pusztai: On the microscopic structure of some aqueous electrolyte solutions *Acta Cryst*. **A 60** (Supplement) S56, (2004) IF: 1.72