

# Todor Dudev

Faculty of Chemistry and Pharmacy

Sofia University

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## Areas of Expertise

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- Computational Chemistry/Biochemistry/Biophysics
- Metals in Biology and Medicine
- Molecular Modeling
- Coordination Chemistry
- Chemoinformatics
- Infrared and Raman Spectroscopy
- Teaching / Course Design

## Education

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### **D. Sc. in Chemistry**

2015, *Sofia University, Bulgaria*

Thesis: "Factors Governing the Processes of Metal Binding and Selectivity in Metalloproteins and Ion Channels: In Silico Investigations"

### **Ph.D. in Chemistry**

1989, *Sofia University, Bulgaria*

Thesis: "Infrared Band Intensity Analysis: Algorithms and Applications"

### **M.Sc. in Chemistry**

1984, *Sofia University, Bulgaria*

Graduated with Honors and received a Gold Medal for outstanding academic performance.

## Academic Positions

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<b>Professor in Chemistry</b>	2013 –
Faculty of Chemistry and Pharmacy Sofia University, Bulgaria	
<b>Senior Research Associate</b>	1997 – 2013
Institute of Biomedical Sciences Academia Sinica, Taiwan	
<b>Associate Professor</b>	1997 – 2000
Department of Chemistry Sofia University, Bulgaria	
<b>Assistant Professor</b>	1989 – 1997
Department of Chemistry Sofia University, Bulgaria	

## Sabbaticals and International Grants

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<b>Visiting Professor</b>	Spring 2014, 2015, 2018
Universidad de Alcala de Henares Alcala de Henares, Spain	
<b>Visiting Professor</b>	Autumn 2012
Laboratoire de Pharmacochimie Moleculaire et Cellulaire University Paris – Descartes Paris, France	
<b>Visiting Scientist</b>	Summer 1999, Autumn 1993
Instituto de Estructura de la Materia Consejo Superior de Investigaciones Cientificas Madrid, Spain	
<b>Visiting Scientist</b>	Summer 1996
College of Arts & Sciences University of Missouri-Kansas City Kansas City, MO, USA	

**Visiting Scientist** Winter 1994, Spring 1996

Department of Analytical Chemistry  
Dresden University of Technology,  
Dresden, Germany

**Visiting Scientist** Summer 1993

Department of Chemistry & Applied Chemistry  
University of Salford,  
Manchester, UK

**Postdoctoral Researcher** 10/1989 – 9/1990

Research Laboratory of Resources Utilization,  
Tokyo Institute of Technology  
Tokyo, Japan

### **Recent Invited Talks**

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- Workshop “Advanced Materials”, Duni, Bulgaria, 2018.
- Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Czech Republic, 2018.
- Departament de Nutricio, Ciencies de l’Alimentacio i Gastronomia, Universitat de Barcelona, Spain, 2017.
- Conference on Modeling Interactions in Biomolecules VIII, Pilsen, Czech Republic, 2017.
- Workshop “Advanced Materials”, Pomorie, Bulgaria, 2017.
- 3<sup>rd</sup> Symposium on Weak Molecular Interactions, Opole, Poland, 2017.
- Department of Chemistry, Jagiellonian University, Krakow, Poland, 2017.
- The Third International Conference on Computational Science and Engineering, Ho Chi Minh City, Vietnam, 2016.
- Department of Organic Chemistry, The Hebrew University of Jerusalem, Israel, 2016.
- Workshop “Advanced Functional Materials”, Pravets, Bulgaria, 2016.
- Tenth Workshop on Biological Activity of Metals, Synthetic Compounds and Natural Products, Sofia, Bulgaria, 2015.
- Unidad Docente de Quimica Fisica, Universidad de Alcala de Henares, Alcala de Henares, Spain, 2014, 2015, 2018.

- Scientific Session of the Faculty of Chemistry and Pharmacy, Sofia University, Sofia, Bulgaria, 2015.
- Workshop “Applied Research on Functional Materials”, Velingrad, Bulgaria, 2014.
- Conference on Modeling Interactions in Biomolecules VI, Marianske Lazne, Czech Republic, 2013.
- Workshop “Fundamental and Applied, Approved and New Research Methods with Biomedical Application”, Pravets, Bulgaria, 2013.
- 17<sup>th</sup> Biophysics Conference, Taipei, Taiwan, 2012.
- Laboratoire de Pharmacochimie Moleculaire et Cellulaire, University Paris – Descartes, France, 2012.
- Structural Bioinformatics Division, Institute Pasteur, Paris, France, 2012
- Laboratoire de Biochimie Theorique, Institute de Biologie Physico-Chimique, Paris, France, 2012.
- Conference on Modeling Interactions in Biomolecules V, Kutna Hora, Czech Republic, 2011.
- Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan, 2011.
- 2<sup>nd</sup> Annual International Conference on Computational and Systems Biology, Hangzhou, China, 2010.
- 1<sup>st</sup> Workshop on Multiscale Simulations of Biological Molecules, Taipei, Taiwan, 2010.
- Conference on Modeling Interactions in Biomolecules IV, Hrubá Skála, Czech Republic, 2009.
- Conference on Viral Membrane Proteins, Heidelberg, Germany, 2008.
- 12<sup>th</sup> International Conference on Theoretical Aspects of Catalysis, Varna, Bulgaria, 2008.
- 3<sup>rd</sup> Asian Pacific Conference on Theoretical and Computational Chemistry, Beijing, China, 2007.
- 3<sup>rd</sup> Humboldt Conference on Computational Chemistry, Varna, Bulgaria, 2006.
- Modeling Interactions in Biomolecules II, Prague, Czech Republic, 2005.
- Modeling Interactions in Biomolecules, Nove Hradky, Czech Republic, 2003.

## **Manuscript Reviewer**

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- Journal of the American Chemical Society
- Journal of Physical Chemistry
- Zeitschrift für Anorganische und Allgemeine Chemie

- Journal of Computer-Aided Molecular Design
- Journal of the Chinese Chemical Society
- Journal of Molecular Modeling
- BioMetals
- Journal of Molecular Graphics and Modeling
- Spectrochimica Acta
- Journal of Molecular Structure
- Metallomics
- Physical Chemistry Chemical Physics
- Journal of Organic Chemistry
- Inorganic Chemistry

**Member of the Editorial Board of the journal "Computational Chemistry"**

**Member of the Editorial Board of the journal "World Journal of Methodology"**

**Member of the Editorial Board of the journal "EUREKA: Life Sciences"**

**Member of the Editorial Advisory Board of the "Handbook of Research on Computational and Systems Biology: Interdisciplinary Applications", IGI Global, 2010**

**External Grant-Proposal Evaluator for the Research Grants Council of Hong Kong**

**Grant-Proposal Evaluator for the European Research Council**

## **Publications**

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One book, 5 book chapters and 99 research papers. *Please refer to the attached list for a complete record of all publications.*

Total number of citations (without self-citations): 2000

H-index: 25

## **Teaching Experience**

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### **University Courses Taught**

2013 - *Ab initio MO Calculations* – Sofia University, Bulgaria

2013 - *Computational Methods in Spectroscopy* – Sofia University, Bulgaria

2013 - *Instrumental Methods in Chemistry* – Sofia University, Bulgaria

2013 - *Pharmaceutical Analysis* – Sofia University, Bulgaria

2015 – *Biochemistry* – Sofia University, Bulgaria

2006 *Protein Biochemistry* – National Yang Ming University, Taiwan

2006 *Medicinal Chemistry* – National Yang Ming University, Taiwan

1991 – 1997 *Applied Spectroscopy* – Sofia University, Bulgaria

1991 – 1997 *Spectroscopy of Biologically Active Molecules* – Sofia University,  
Bulgaria

1987 – 1997 *Quantum Chemistry and Spectroscopy* – Sofia University, Bulgaria

### **Distance Learning**

Pioneered distance learning in Bulgaria together with a team of other Sofia University researches. Worked as a member of the National Contact Point, National Centre for Distance Education, Subcontractor for Bulgaria of the PHARE Multi-Country Program for Distance Education, 1995-1997. Developed distance learning programs, materials and methodologies that were among the first in Eastern Europe.

## List of Publications

### Book

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B. Galabov and T. Dudev, "Vibrational Intensities", Elsevier, Amsterdam, 1996 (342 pages).

### Book Chapters

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C. Lim and T. Dudev, "Potassium Versus Sodium Selectivity in Monovalent Ion Channel Selectivity Filters" in *The Alkali Metal Ions: Their Role for Life*, Vol. 16 of Metal Ions in Life Sciences (Eds. A. Sigel, H. Sigel, R.K.O. Sigel), Springer International, Cham, Switzerland, 2016, pp. 325-347.

T. Dudev and C. Lim, "Calcium Ion Selectivity in Biological Systems", in *Encyclopedia of Metalloproteins* (V.N. Uversky, R.H. Kretsinger, E.A. Permyakov, Eds.), Springer Science, New York, 2013, pp. 478-484.

T. Kamisuki, T. Dudev and C. Hirose, "Transient Resonance CARS Study on Photoionization of Shorter Diphenylpolyenes in Various Polar Solvents", in *Time-Resolved Vibrational Spectroscopy V* (H. Takahashi, Ed.), Springer-Verlag, Berlin, 1992, pp. 141-144.

B. Galabov, T. Dudev and J.R. Durig, "Molecular Conformation from Vibrational Intensity Analysis", in *Progress in Molecular Spectroscopy* (R. Salzer, H. Kriegsmann, G. Werner, Eds.), Teubner, Leipzig, 1988, p. 113.

B. Galabov, T. Dudev and J.R. Durig, "Bond Properties and Molecular Conformation from Vibrational Intensity Analysis", in *State-of-the-art in Vibrational Spectroscopy* (Z. Meic, Ed.), Amsterdam, 1989, p. 569.

- *Reviews*

1. N. Kircheva and T. Dudev, "Mechanism of therapeutic action of abiogenic Li<sup>+</sup> and Ga<sup>3+</sup> ions: Insights from theoretical studies", *Bulg. Chem. Commun.* **50** (2018) 55-62.
2. T. Dudev and C. Lim, "Competition among Metal Ions for Protein Binding Sites: Determinants of Metal Ion Selectivity in Proteins", *Chem. Rev.* **114** (2014) 538-556.
3. D. Meffre, J. Grenier, S. Bernard, F. Courtin, T. Dudev, G.G. Shackleford, M. Jafarian-Tehrani and C. Massaad, "Wnt and Lithium: a Common Destiny in the Therapy of Nervous System Pathologies?", *Cell. Mol. Life Sci.* **71** (2014) 1123-1148.
4. T. Dudev and C. Lim, "Ion Selectivity Strategies of Sodium Channel Selectivity Filters", *Acc. Chem. Res.* **47** (2014) 3580-3587.
5. T. Dudev and C. Lim, "Metal Binding and Selectivity in Metalloproteins: Insights from Computational Studies", *Annual Review of Biophysics* **37** (2008) 97-116.
6. T. Dudev and C. Lim, "Effect of Carboxylate-Binding Mode on Metal Binding/Selectivity and Function in Proteins", *Acc. Chem. Res.* **40** (2007) 85-93.
7. T. Dudev and C. Lim, "Principles Governing Mg, Ca and Zn Selectivity in Proteins", *Chem. Rev.* **103** (2003) 773 – 787.
8. T. Dudev and C. Lim, "Metal Binding and Selectivity in Zinc Proteins", *J. Chin. Chem. Soc.* **50** (2003) 1093-1102.

- *Journal Articles*

9. K. Mazmanian, T. Dudev and C. Lim, "How first shell – second shell interactions and metal substitution modulate protein function", *Inorg. Chem.* **57** (2018) DOI: 10.1021/acs.inorgchem.8b01029.
10. S. Angelova, V. Nikolova and T. Dudev, "Divalent metal ions binding to lactose: a DFT computational study", *Bulg. Chem. Commun.* **50** (2018) 130-134.
11. D. Cheshmedzhieva, N. Toshev, M. Gerova, O. Petrov and T. Dudev, "Sulfur and selenium derivatives of suberoyl anilide hydroxamic acid (SAHA) as a plausible HDAC inhibitors: a DFT study of their tautomerism and metal affinity/selectivity", *Bulg. Chem. Commun.* **50** (2018) 228-236.



12. T. Dudev, C. Grauffel, S.-T. D. Hsu and C. Lim, "How native and non-native cations bind and modulate the properties of GTP/ATP", *J. Chem. Theor. Comput.* **14** (2018) 3311-3320.
13. T. Dudev, K. Mazmanian and C. Lim, "Competition between  $\text{Li}^+$  and  $\text{Na}^+$  in sodium transporters and receptors: Which  $\text{Na}^+$ -binding sites are "therapeutic"  $\text{Li}^+$  targets?", *Chem. Sci.* **9** (2018) 4093-4103.
14. D. Cheshmedzhieva, N. Toshev, M. Gerova, O. Petrov and T. Dudev, "Hydroxamic acid derivatives as histone deacetylase inhibitors: a DFT study of their tautomerism and metal affinities/selectivities", *J. Mol. Modeling* **24** (2018) 114.
15. T. Dudev, D. Cheshmedzhieva and L. Doudeva, "Competition between abiogenic  $\text{Al}^{3+}$  and native  $\text{Mg}^{2+}$ ,  $\text{Fe}^{2+}$  and  $\text{Zn}^{2+}$  ions in protein binding sites: Implications for aluminium toxicity", *J. Mol. Modeling* **24** (2018) 55.
16. S. Angelova, V. Nikolova, S. Pereva, T. Spassov and T. Dudev, " $\alpha$ -Cyclodextrin: How Effectively Can Its Hydrophobic Cavity Be Hydrated?", *J. Phys. Chem. B* **121** (2017) 9260-9267.
17. V. Nikolova, S. Angelova and T. Dudev, "IIA/IIB group metal cations hosted by  $\beta$ -cyclodextrin: a DFT study", *Bulg. Chem. Commun.* **49** (2017) 189-194.
18. S.E. Angelova, V.K. Nikolova and T.M. Dudev, "Determinants of the host-guest interactions between  $\alpha$ -,  $\beta$ - and  $\gamma$ -cyclodextrins and group IA, IIA and IIIA metal cations: a DFT/PCM study", *Phys. Chem. Chem. Phys.* **19** (2017) 15129-15136.
19. S. Angelova, V. Nikolova, N. Molla and T. Dudev, "Factors Governing the Host-Guest Interactions between IIA/IIB Group Metal Cations and  $\alpha$ -Cyclodextrin: A DFT/CDM Study", *Inorg. Chem.* **56** (2017) 1981-1987.
20. T. Dudev, C. Grauffel and C. Lim, "How Native and Alien Metal Cations Bind ATP: Implications for Lithium as a Therapeutic Agent", *Sci. Rep.* **7** (2017) 42377.
21. T. Dudev and L. Doudeva, "How the extra methylene group affects the ligation properties of Glu vs. Asp and Gln vs. Asn amino acids: a DFT/PCM study", *J. Mol. Modeling* **23** (2017) 45.
22. T. Dudev and V. Nikolova, "Determinants of  $\text{Fe}^{2+}$  over  $\text{M}^{2+}$  ( $\text{M} = \text{Mg}, \text{Mn}, \text{Zn}$ ) Selectivity in Non-Heme Iron Proteins", *Inorg. Chem.* **55** (2016) 12644-12650.
23. K. Mazmanian, K. Sargsyan, C. Grauffel, T. Dudev, and C. Lim, "Preferred Hydrogen-Bonding Partners of Cysteine: Implications for Regulating Cys Functions", *J. Phys. Chem. B* **120** (2016) 10288-10296.

24. T. Dudev, C. Grauffel and C. Lim, "Influence of the Selectivity Filter Properties on Proton Selectivity in the Influenza A M2 Channel", *J. Am. Chem. Soc.* **138** (2016) 13038-13047.
25. T. Dudev, K. Mazmanian, and C. Lim, "Factors controlling the selectivity for Na<sup>+</sup> over Mg<sup>2+</sup> in sodium transporters and enzymes", *Phys. Chem. Chem. Phys.* **18** (2016) 16986-16997.
26. V. Nikolova, S. Angelova, N. Markova, and T. Dudev, "Gallium as a Therapeutic Agent: A Thermodynamic Evaluation of the Competition between Ga<sup>3+</sup> and Fe<sup>3+</sup> Ions in Metalloproteins", *J. Phys. Chem. B* **120** (2016) 2241-2248.
27. S. Pereva, T. Himitliiska, T. Spassov, S.D. Stoyanov, L.N. Arnaudov and T. Dudev, "Cyclodextrin-Based Solid-Gas Clathrates", *J. Agric. Food Chem.* **63** (2015) 6603-6613.
28. T. Dudev, B. Musset, D. Morgan, V.V. Cherny, S.M.E. Smith, K. Mazmanian, T.E. DeCoursey and C. Lim, "Selectivity Mechanism of the Voltage-gated Proton Channel, Hv1", *Sci. Rep.* **5** (2015) 10320.
29. T. Dudev and C. Lim, "Ion Selectivity in the Selectivity Filters of Acid-Sensing Ion Channels", *Sci. Rep.* **5** (2015) 7864.
30. T. Dudev, M. Devereux, M. Meuwly, C. Lim, J.-P. Piquemal and N. Gresh, "Quantum-Chemistry Based Calibration of the Alkali Metal Cation Series (Li<sup>+</sup>-Cs<sup>+</sup>) for Large-Scale Polarizable Molecular Mechanics/Dynamics Simulations", *J. Comp. Chem.* **36** (2015) 285-302.
31. C.S. Babu, Y.-M. Lee, T. Dudev and C. Lim, "Modeling Zn<sup>2+</sup> Release from Metallothionein", *J. Phys. Chem. A* **118** (2014) 9244-9252.
32. T. Dudev, "Modeling Metal Binding Sites in Proteins by Quantum Chemical Calculations", *Comp. Chem.* **2** (2014) 19-21.
33. T. Dudev and C. Lim, "Evolution of Eukaryotic Ion Channels: Principles Underlying the Conversion of Ca<sup>2+</sup>-Selective to Na<sup>+</sup>-Selective Channels", *J. Am. Chem. Soc.* **136** (2014) 3553-3559.
34. T. Dudev and C. Lim, "Importance of Metal Hydration on the Selectivity of Mg<sup>2+</sup> vs. Ca<sup>2+</sup> in Magnesium Ion Channels", *J. Am. Chem. Soc.* **135** (2013) 17200-17208.
35. C.S. Babu, T. Dudev and C. Lim, "Differential role of the protein matrix on the binding of a catalytic aspartate to Mg<sup>2+</sup> vs. Ca<sup>2+</sup>: Application to Ribonuclease H", *J. Am. Chem. Soc.* **135** (2013) 6541-6548.

36. T. Dudev and C. Lim, "Competition among  $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$ , and  $\text{Na}^+$  for Model Ion Channel Selectivity Filters: Determinants of Ion Selectivity", *J. Phys. Chem. B* **116** (2012) 10703-10714.
37. T. Dudev and C. Lim, "Why Voltage-Gated  $\text{Ca}^{2+}$  and Bacterial  $\text{Na}^+$  Channels with the Same EEEE Motif in Their Selectivity Filters Confer Opposite Metal Selectivity", *Phys. Chem. Chem. Phys.* **14** (2012) 12451-12456.
38. T. Dudev and C. Lim, "The Effect of Metal Binding on the Characteristic Infrared Band Intensities of Ligands of Biological Interest", *J. Mol. Struct.* **1009** (2012) 83-88.
39. T. Dudev and C. Lim, "Competition Between  $\text{Li}^+$  and  $\text{Mg}^{2+}$  in Metalloproteins. Implications for Lithium Therapy", *J. Am. Chem. Soc.* **133** (2011) 9506-9515.
40. T. Dudev and C. Lim, "Factors Controlling the Mechanism of  $\text{NAD}^+$  NonRedox Reactions", *J. Am. Chem. Soc.* **132** (2010) 16533-16543.
41. T. Dudev and C. Lim, "Factors Governing the  $\text{Na}^+$  vs  $\text{K}^+$  Selectivity in Sodium Ion Channels", *J. Am. Chem. Soc.* **132** (2010) 2321-2332.  
Video abstract: <http://pubs.acs.org/JACSbeta/scivee/index.html#video3>
42. T. Dudev and C. Lim, "Metal Binding Affinity and Selectivity of Nonstandard Natural Amino Acid Residues from DFT/CDM Calculations", *J. Phys. Chem. B* **113** (2009) 11754-11764.
43. T. Dudev and C. Lim, "Determinants of  $\text{K}^+$  vs.  $\text{Na}^+$  Selectivity in Potassium Channels", *J. Am. Chem. Soc.* **131** (2009) 8092-8101.
44. T.-Y. Yang, T. Dudev and C. Lim, "Mononuclear versus Binuclear Metal Binding Sites: Metal Binding Affinity and Selectivity from PDB Survey and DFT/CDM Calculations", *J. Am. Chem. Soc.* **130** (2008) 3844-3852.
45. T. Dudev and C. Lim, "All-Electron Calculations of the Nucleation Structures in Metal-Induced Zinc-Finger Folding: Role of the Peptide Backbone", *J. Am. Chem. Soc.* **129** (2007) 12497-12504.
46. T. Dudev and C. Lim, "Competition between Protein Ligands and Cytoplasmic Inorganic Anions for the Metal Cation: A DFT/CDM Study", *J. Am. Chem. Soc.* **128** (2006) 10541-10548.

47. M. Dudev, J. Wang, T. Dudev and C. Lim, "Factors Governing the Metal Coordination Number in Metal Complexes from Cambridge Structural Database Analysis", *J. Phys. Chem. B* **110** (2006) 1889-1895.
48. T. Dudev and C. Lim, "A DFT/CDM Study of Metal-Carboxylate Interactions in Metalloproteins: Factors Governing the Maximum Number of Metal-bound Carboxylates", *J. Am. Chem. Soc.* **128** (2006) 1553-1561.
49. T. Dudev, L-Y. Chang and C. Lim, "Factors Governing the Substitution of  $\text{La}^{3+}$  for  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$  in Metalloproteins: A DFT/CDM Study", *J. Am. Chem. Soc.* **127** (2005) 4091-4103.
50. T. Dudev and C. Lim, "Oxyanion Selectivity in Sulfate and Molybdate Transport Proteins: An Ab Initio/CDM Study", *J. Am. Chem. Soc.* **126** (2004) 10296-10305.
51. T. Dudev and C. Lim, "Monodentate vs. Bidentate Carboxylate Binding in Magnesium and Calcium Proteins: What are the Basic principles", *J. Phys. Chem. B* **108** (2004) 4546-4557.
52. C.S. Babu, T. Dudev, R. Casareno, J.A. Cowan and C. Lim, "A Combined Experimental and Theoretical Study of Divalent Metal Ion Selectivity and Function in Proteins: Application to *E. coli* Ribonuclease H1", *J. Am. Chem. Soc.* **125** (2003) 9318-9328.
53. T. Dudev, Y-I. Lin, M. Dudev and C. Lim, "First-Second Shell Interactions in Metal Binding Sites in Proteins: A PDB Survey and DFT/CDM Calculations", *J. Am. Chem. Soc.* **125** (2003) 3168 – 3180.
54. T. Dudev and C. Lim, "Factors Governing the Protonation State of Cysteines in Proteins: An Ab Initio/CDM Study", *J. Am. Chem. Soc.* **124** (2002) 6759 – 6766.
55. R. Escribano, J.J. Sloan, N. Siddique, N. Sze and T. Dudev, "Raman Spectroscopy of Carbon-Containing Particles", *Vibr. Spectrosc.* **26** (2001) 179 – 186.
56. T. Dudev and C. Lim, "Modeling  $\text{Zn}^{2+}$ -Cysteinate Complexes in Proteins", *J. Phys. Chem. B* **105** (2001) 10709-10714.
57. S. Ilieva, B. Galabov, T. Dudev, T. Gounev and J.R. Durig, "Effective bond charges from infrared intensities in  $\text{CH}_4$ ,  $\text{SiH}_4$ ,  $\text{GeH}_4$  and  $\text{SnH}_4$ ", *J. Mol. Struct.* **565-566** (2001) 395 – 398.

58. T. Dudev and C. Lim, "Metal selectivity in metalloproteins: Zn<sup>2+</sup> vs. Mg<sup>2+</sup>", *J. Phys. Chem. B* **105** (2001) 4446 – 4452.
59. B. Galabov, T. Dudev and S. Ilieva, "The Creation of Intensity Theory in Vibrational Spectroscopy: Key Role of Ab Initio Quantum Mechanical Calculations", *Annu. Univ. Sofia - Fac. Chemie* **91** (2001) 171 – 183.
60. T. Dudev and C. Lim, "Tetrahedral vs. octahedral Zn<sup>2+</sup> complexes with ligands of biological interest: a DFT/CDM study", *J. Am. Chem. Soc.* **122** (2000) 11146 – 11153.
61. G.H. Hakimelahi, A.A. Moosavi-Movahedi, S-C. Tsay, F-Y. Tsay, J.D. Wright, T. Dudev, S. Hakimelahi and C. Lim, "Design, synthesis and structure-activity relationship of novel carbapenem antibiotics with high stability to Xanthomonas Maltophilia Oxyiminocephalosporinase Type II", *J. Med. Chem.* **43** (2000) 3632-3640.
62. T. Dudev and C. Lim, "Metal binding in proteins: the effect of the dielectric medium", *J. Phys. Chem. B* **104** (2000) 3692 - 3694.
63. T. Dudev and C. Lim, "Incremental binding free energies in Mg<sup>2+</sup> complexes: a DFT study", *J. Phys. Chem. A* **103** (1999) 8093 - 8100.
64. T. Dudev, J.A. Cowan and C. Lim, "Competitive binding in magnesium coordination chemistry: water versus ligands of biological interest", *J. Am. Chem. Soc.* **121** (1999) 7665 - 7673.
65. I. Petkov, T. Dudev, N. Sertova, T. Deligeorgiev and V. Drjanska, "Photoinduced protonation of dyes in polymer matrix. Novel effective mode for conversion and storage of solar energy. Theoretical approach for predicting the light energy storage efficiency" (1999) *Emedia Science Ltd., Virtual conferences: Internet Science publishing* <http://www.photobiology.com/reviews/default.htm>
66. W.B. Fischer, I. Unverricht, T. Dudev and R. Salzer, "Negative ions causing structural changes of the acetylcholine cation – FTIR spectroscopy and theoretical calculations", *Asian J. Spectrosc.* **2** (1998) 125 - 130.
67. B. Galabov, T. Dudev, S. Ilieva and J.R. Durig, "Creation of intensity theory in vibrational spectroscopy: key role of ab initio quantum chemical calculations", *Int. J. Quant. Chem.* **70** (1998) 331 - 339.

68. T. Dudev and C. Lim, "Ring strain energies from ab initio calculations", *J. Am. Chem. Soc.* **120** (1998) 4450 - 4458.
69. T. Dudev, P. Bobadova-Parvanova, D. Pencheva and B. Galabov, "Molecular geometry, vibrational frequencies, infrared intensities and C<sup>o</sup>N effective bond charges in a series of simple nitrile compounds: HF/6-31+G(d,p) MO study", *J. Mol. Struct.* **436/437** (1997) 427 - 433.
70. B. Galabov, T. Dudev and S. Ilieva, "Effective bond charges from infrared and Raman intensities", *J. Mol. Struct.* **408/409** (1997) 57 - 62.
71. B. Galabov, P. Bobadova-Parvanova and T. Dudev, "Interpretation of carbonyl stretching band intensities in the infrared spectra: an ab initio MO study", *J. Mol. Struct.* **406** (1997) 119 - 125.
72. B. Galabov, S. Ilieva, B. Hadjieva and T. Dudev, "N-H stretching frequencies and conformation of substituted ureas: an ab initio MO study", *J. Mol. Struct.* **407** (1997) 47 - 51.
73. T. Dudev and B. Galabov, "Ab initio calculations of Raman intensity parameters and geometry of polyynes and polyynenitriles", *Spectrochim. Acta* **53A** (1997) 2053 - 2059.
74. V. Koleva, T. Dudev and I. Wawer, "<sup>1</sup>H and <sup>13</sup>C NMR study and AM1 calculations of some azobenzenes and N-benzylideneanilines: effect of substituents on the molecular planarity", *J. Mol. Struct.* **412** (1997) 153 - 159.
75. T. Dudev, "Predicted Raman intensities of CH<sub>3</sub>CCH, CH<sub>3</sub>CCD, CD<sub>3</sub>CCH, CD<sub>3</sub>CCD and <sup>12</sup>CH<sub>3</sub><sup>13</sup>C<sup>13</sup>CH", *J. Raman Spectrosc.* **28** (1997) 199 - 204.
76. T. Dudev and B. Galabov, "Interpretation of Raman intensities: effective induced bond charges from atomic polarizability tensors", *Spectrochim. Acta* **52A** (1996) 527 - 538.
77. S. Ilieva, M. Krusteva, T. Dudev, B. Galabov, T. Gounev and J.R. Durig, "Effective bond charges from infrared intensities: ab initio calculations", *J. Mol. Struct.* **377** (1996) 75 - 79.
78. S. Metsov, T. Dudev and V. Koleva, "Infrared and NMR study of some 2-styrylindolium dyes", *J. Mol. Struct.* **350** (1995) 241 - 246.

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