Todor Dudev

Faculty of Chemistry and Pharmacy

Sofia University

1 James Bourchier Avenue

1164 Sofia, Bulgaria

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Areas of Expertise

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

Degrees

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

Professor in Chemistry 2013 –
Faculty of Chemistry and Pharmacy
Sofia University, Bulgaria

Senior Research Associate 1997 – 2013
Institute of Biomedical Sciences
Academia Sinica, Taiwan

Associate Professor 1997 – 2000
Department of Chemistry
Sofia University, Bulgaria

Assistant Professor 1989 – 1997
Department of Chemistry
Sofia University, Bulgaria

Sabbaticals and International Grants

Visiting Professor Spring 2014, 2015, 2018
Universidad de Alcala de Henares
Alcala de Henares, Spain

Visiting Professor Autumn 2012
Laboratoire de Pharmacochimie Moleculaire et Cellulaire
University Paris – Descartes
Paris, France

Visiting Scientist Summer 1999, Autumn 1993
Instituto de Estructura de la Materia
Consejo Superior de Investigaciones Cientificas
Madrid, Spain

Visiting Scientist 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

Invited Talks

- 27th Lecture Session on Modern Directions of Natural Sciences, Sofia University, Bulgaria, 2021.
- Workshop "Advanced Materials", St.St. Constantine and Helena, Bulgaria, 2019.
- PRACE Winter School 2018 – Computational Chemistry, Biochemistry and Medicinal Chemistry – Methods and Tools, Sofia, Bulgaria, 2018.
- The 13th Workshop with International Participation: Biological Activity of Metals, Synthetic Compounds and Natural Products, Sofia, Bulgaria, 2018.
- 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.
- 3rd 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.
- 17th 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.
- 2nd Annual International Conference on Computational and Systems Biology, Hangzhou, China, 2010.
- 1st Workshop on Multiscale Simulations of Biological Molecules, Taipei, Taiwan, 2010.
- Conference on Modeling Interactions in Biomolecules IV, Hruba Skala, Czech Republic, 2009.
- Conference on Viral Membrane Proteins, Heidelberg, Germany, 2008.
- 12th International Conference on Theoretical Aspects of Catalysis, Varna, Bulgaria, 2008.
- 3rd Asian Pacific Conference on Theoretical and Computational Chemistry, Beijing, China, 2007.
- 3rd Humboldt Conference on Computational Chemistry, Varna, Bulgaria, 2006.
- Modeling Interactions in Biomolecules II, Prague, Czech Republic, 2005.

- Modeling Interactions in Biomolecules, Nove Hrady, Czech Republic, 2003.
- XXIII European Congress on Molecular Spectroscopy, Balatonfured, Hungary, 1996

Manuscript Reviewer

- Journal of the American Chemical Society
- Journal of Physical Chemistry
- Zeitschrift fur 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 "Frontiers in Pharmacology"

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

Member of the Editorial Board of "International Journal of Molecular Sciernces"

Grant-Proposal Evaluator for the European Research Council

Awards: "Pythagoras" award for exceptional achievements in the field of natural and engineering sciences (Bulgaria, 2017)

Publications

One book, 3 book chapters and 124 research papers. *Please refer to the attached list for a complete record of all publications.*

Total number of citations (without self-citations): 3300

Total impact factor: 740

H-index: 29 (WoS) and 32 (Google Scholar)

Teaching Experience

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.

Todor Dudev

List of Publications

Book

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

Book Chapters

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.

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.

Papers

- *Reviews*

1. T. Dudev, C. Grauffel and C. Lim, “Calcium in Signaling: Its Specificity and Vulnerabilities toward Biogenic and Abiogenic Metal Ions”, *J. Phys. Chem. B* **125** (2021) 10419-10431.

2. N. Kircheva and T. Dudev, „Competition between abiogenic and biogenic metal cations in biological systems: Mechanisms of gallium‘s anticancer and antibacterial effect“, *J. Inorg. Biochem.* **214** (2021) 111309.

3. T. Dudev, K. Mazmanian, W.-H. Weng, C. Grauffel and C. Lim, “Free and bound lithium in brain signaling“, *Acc. Chem. Res*. **52** (2019) 2960-2970.

4. N. Kircheva and T. Dudev, “Mechanism of therapeutic action of abiogenic Li^+ and Ga^{3+} ions: Insights from theoretical studies”, *Bulg. Chem. Commun*. **50** (2018) 55-62.

5. 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.

6. 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.

7. T. Dudev and C. Lim, “Ion Selectivity Strategies of Sodium Channel Selectivity Filters”, *Acc. Chem. Res.* **47** (2014) 3580-3587.

8. T. Dudev and C. Lim, “Metal Binding and Selectivity in Metalloproteins: Insights from Computational Studies”, *Annual Review of Biophysics* **37** (2008) 97-116.

9. 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.

10. T. Dudev and C. Lim, “Principles Governing Mg, Ca and Zn Selectivity in Proteins”, *Chem. Rev.* **103** (2003) 773 – 787.

11. T. Dudev and C. Lim, “Metal Binding and Selectivity in Zinc Proteins”, *J. Chin. Chem. Soc.* **50** (2003) 1093-1102.

- *Journal Articles*

12. D. Cheshmedzhieva, S. Ilieva, E.A. Permyakov, S.E. Permyakov and T. Dudev, „Ca^{2+}/Sr^{2+} Selectivity in Calcium-Sensing Receptor (CaSR): Implications for Strontium’s Anti-Osteoporosis Effect“, *Biomolecules* **11** (2021) 1576.

13. A.A. Vologzhannikova, M.P. Shevelyova, A.S. Kazakov, A.S. Sokolov, N.I. Borisova, E. A. Permyakov, N. Kircheva, V. Nikolova, T. Dudev and S.E. Permyakov, “Strontium Binding to α-Parvalbumin, a Canonical Calcium-Binding Protein of the “EF-Hand” Family”, *Biomolecules* **11** (2021) 1158.

14. C. Grauffel, W.-H. Weng, T. Dudev, and C. Lim, "The Trinuclear Calcium Site in the C2 domain of PKCα/γ is Prone to Lithium Attack", *ACS Omega* **6** (2021) 20657-20666.

15. N. Toshev, D. Cheshmedzhieva and T. Dudev, "Factors governing the affinity and selectivity of histone deacetylase inhibitors for the HDAC8 enzyme active site: Implications for anticancer therapy", *J. Phys. Org. Chem.* **34** (2021) e4268.

16. D. Damyanov, V. Nikolova, S. Angelova and T. Dudev, "Halide anion solvation and recognition by bambusurils: a DFT study", *J. Mol. Liq.* **335** (2021) 116160.

17. C. Grauffel, T. Dudev and C. Lim, "Metal Affinity/Selectivity of Monophosphate-Containing Signaling/Lipid Molecules", *J. Chem. Theor. Comput*. **17** (2021) 2444-2456.

18. V. Nikolova, A. Velinova, S. Dobrev, N. Kircheva, S. Angelova and T. Dudev, "Host−Guest Complexation of Cucurbit[7]Uril and Cucurbit[8]Uril with the Antineoplastic and Multiple Sclerosis Agent Mitoxantrone (Novantrone)", *J. Phys. Chem. A* **125** (2021) 536-542.

19. N. Kircheva, S. Dobrev, V. Nikolova, S. Angelova, and T. Dudev, "Zinc and Its Critical Role in Retinitis pigmentosa: Insights from DFT/SMD Calculations", *Inorg. Chem*. **59** (2020) 17347-17355.

20. N. Kircheva, S. Dobrev, L. Dasheva, I. Koleva, V. Nikolova, S. Angelova and T. Dudev, "Complexation of biologically essential (mono- and divalent) metal cations to cucurbiturils: A DFT/SMD evaluation of the key factors governing the host-guest recognition", *RSC Advances* **10** (2020) 28139-28147.

21. S. Yordanova-Tomova, D. Cheshmedzhieva, S. Stoyanov, T. Dudev and I. Grabchev, „Synthesis, Photophysical Characterization, and Sensor Activity of new 1,8-Naphtalimide Derivatives", *Sensors* **20** (2020) 3892.

22. N. Kircheva and T. Dudev, "Gallium as an Antibacterial Agent: A DFT/SMD Study of the Ga^{3+}/Fe^{3+} Competition for Binding Bacterial Siderophores", *Inorg. Chem*. **59** (2020) 6242-6254.

23. T. Dudev, D. Cheshmedzhieva, R. Dimitrova, P. Dorkov and I. Pantcheva, "Factors governing the competition between group IA and IB cations for monensin A: a DFT/PCM study", *RSC Advances* **10** (2020) 5734-5741.

24. T. Dudev, L.M. Frutos and O. Castano, "How mechanical forces can modulate the metal affinity and selectivity of metal binding sites in proteins", *Metallomics* **12** (2020) 363-370.

25. S. Pereva, V. Nikolova, T. Sarafska, S. Angelova, T. Spassov, T. Dudev, "Inclusion complexes of ibuprofen and β-cyclodextrin: Supramolecular structure and stability", *J. Mol. Struct*. **1205** (2020) 127575.

26. C. Grauffel, T. Dudev and C. Lim, „Why Cellular Di/Triphosphates Preferably Bind Mg^{2+} and Not Ca^{2+}, *J. Chem. Theor. Comput*. **15** (2019) 6992-7003.

27. S. Ilieva, D. Cheshmedzhieva and T. Dudev, "Electric field influence on the helical structure of peptides: insights from DFT/PCM computations", *Phys. Chem. Chem. Phys*. **21** (2019) 16198-16206.

28. S. Pereva, V. Nikolova, S. Angelova, T. Spassov and T. Dudev, "Water inside β-cyclodextrin cavity: amount, stability and mechanism of binding", *Beilstein J. Org. Chem*. **15** (2019) 1592-1600.

29. N. Kircheva and T. Dudev, "Novel insights into gallium's mechanism of therapeutic action: a DFT/PCM study of the interaction between Ga^{3+} and ribonucleotide reductase substrates", *J. Phys. Chem. B* **123** (2019) 5444-5451.

30. V.K. Nikolova, C.V. Kirkova, S.E. Angelova and T.M. Dudev, "Host-guest interactions between p-sulfonatocalix[4]arene and p-sulfonatothiacalix[4]arene and group IA, IIA and f-block metal cations: a DFT/SMD study", *Beilstein J. Org. Chem.* **15** (2019) 1321-1330.

31. T. Dudev, C. Grauffel and C. Lim, "How Pb^{2+} Binds and Modulates Properties of Ca^{2+}-Signaling Proteins", *Inorg. Chem.* **57** (2018) 14798-14809.

32. T. Dudev, S. Ilieva and L. Doudeva, "How an electric field can modulate the metal ion selectivity of protein binding sites: insights from DFT/PCM calculations", *Phys. Chem. Chem. Phys*. **20** (2018) 24633-24640.

33. K. Mazmanian, T. Dudev and C. Lim, "How first shell – second shell interactions and metal substitution modulate protein function", *Inorg. Chem*. **57** (2018) 14052-14061.

34. S. Angelova, V. Nikolova and T. Dudev, "Divalent metal ions binding to lactose: a DFT computational study", *Bulg. Chem. Commun*. **50** (2018) 130-134.

35. 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.

36. 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.

37. T. Dudev, K. Mazmanian and C. Lim, "Competition between Li^+ and Na^+ in sodium transporters and receptors: Which Na^+-binding sites are "therapeutic" Li^+ targets?", *Chem. Sci.* **9** (2018) 4093-4103.

38. 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.

39. T. Dudev, D. Cheshmedzhieva and L. Doudeva, "Competition between abiogenic Al^{3+} and native Mg^{2+}, Fe^{2+} and Zn^{2+} ions in protein binding sites: Implications for aluminium toxicity", *J. Mol. Modeling* **24** (2018) 55.

40. S. Angelova, V. Nikolova, S. Pereva, T. Spassov and T. Dudev, "α-Cyclodextrin: How Effectively Can Its Hydrophobic Cavity Be Hydrated?", *J. Phys. Chem. B* **121** (2017) 9260-9267.

41. V. Nikolova, S. Angelova and T. Dudev, "IIA/IIB group metal cations hosted by β-cyclodextrin: a DFT study", *Bulg. Chem. Commun*. **49** (2017) 189-194.

42. S.E. Angelova, V.K. Nikolova and T.M. Dudev, "Determinants of the host-guest interactions between α-, β- and γ-cyclodextrins and group IA, IIA and IIIA metal cations: a DFT/PCM study", *Phys. Chem. Chem. Phys.* **19** (2017) 15129-15136.

43. S. Angelova, V. Nikolova, N. Molla and T. Dudev, "Factors Governing the Host−Guest Interactions between IIA/IIB Group Metal Cations and α-Cyclodextrin: A DFT/CDM Study", *Inorg. Chem*. **56** (2017) 1981-1987.

44. 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.

45. 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.

46. T. Dudev and V. Nikolova, "Determinants of Fe^{2+} over M^{2+} (M = Mg, Mn, Zn) Selectivity in Non-Heme Iron Proteins", *Inorg. Chem.* **55** (2016) 12644–12650.

47. 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.

48. 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.

49. T. Dudev, K. Mazmanian, and C. Lim, "Factors controlling the selectivity for Na^+ over Mg^{2+} in sodium transporters and enzymes", *Phys. Chem. Chem. Phys.* **18** (2016) 16986-16997.

50. V. Nikolova, S. Angelova, N. Markova, and T. Dudev, "Gallium as a Therapeutic Agent: A Thermodynamic Evaluation of the Competition between Ga^{3+} and Fe^{3+} Ions in Metalloproteins", *J. Phys. Chem. B* **120** (2016) 2241-2248.

51. 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.

52. 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, H_V1", *Sci. Rep.* **5** (2015) 10320.

53. T. Dudev and C. Lim, "Ion Selectivity in the Selectivity Filters of Acid-Sensing Ion Channels", *Sci. Rep.* **5** (2015) 7864.

54. 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^+-Cs^+) for Large-Scale Polarizable Molecular Mechanics/Dynamics Simulations", *J. Comp. Chem.* **36** (2015) 285-302.

55. C.S. Babu, Y.-M. Lee, T. Dudev and C. Lim, "Modeling Zn^{2+} Release from Metallothionein", *J. Phys. Chem. A* **118** (2014) 9244-9252.

56. T. Dudev, "Modeling Metal Binding Sites in Proteins by Quantum Chemical Calculations", *Comp. Chem*. **2** (2014) 19-21.

57. T. Dudev and C. Lim, "Evolution of Eukaryotic Ion Channels: Principles Underlying the Conversion of Ca^{2+}-Selective to Na^{+}-Selective Channels", *J. Am. Chem. Soc*. **136** (2014) 3553-3559.

58. T. Dudev and C. Lim, "Importance of Metal Hydration on the Selectivity of Mg^{2+} vs. Ca^{2+} in Magnesium Ion Channels", *J. Am. Chem. Soc.* **135** (2013) 17200-17208.

59. C.S. Babu, T. Dudev and C. Lim, "Differential role of the protein matrix on the binding of a catalytic aspartate to Mg^{2+} vs. Ca^{2+}: Application to Ribonuclease H", *J. Am. Chem. Soc*. **135** (2013) 6541-6548.

60. T. Dudev and C. Lim, "Competition among Ca^{2+}, Mg^{2+}, and Na^{+} for Model Ion Channel Selectivity Filters: Determinants of Ion Selectivity", *J. Phys. Chem. B* **116** (2012) 10703-10714.

61. T. Dudev and C. Lim, "Why Voltage-Gated Ca^{2+} and Bacterial Na^{+} Channels with the Same EEEE Motif in Their Selectivity Filters Confer Opposite Metal Selectivity", *Phys. Chem. Chem. Phys.* **14** (2012) 12451-12456.

62. 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.

63. T. Dudev and C. Lim, "Competition Between Li^{+} and Mg^{2+} in Metalloproteins. Implications for Lithium Therapy", *J. Am. Chem. Soc*. **133** (2011) 9506-9515.

64. T. Dudev and C. Lim, "Factors Controlling the Mechanism of NAD^{+} NonRedox Reactions", *J. Am. Chem. Soc*. **132** (2010) 16533-16543.

65. T. Dudev and C. Lim, "Factors Governing the Na^{+} vs 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

66. 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.

67. T. Dudev and C. Lim, "Determinants of K^{+} vs. Na^{+} Selectivity in Potassium Channels", *J. Am. Chem. Soc.* **131** (2009) 8092-8101.

68. 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.

69. 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.

70. 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.

71. 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.

72. 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.

73. T. Dudev, L-Y. Chang and C. Lim, "Factors Governing the Substitution of La^{3+} for Ca^{2+} and Mg^{2+} in Metalloproteins: A DFT/CDM Study", *J. Am. Chem. Soc.* **127** (2005) 4091-4103.

74. 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.

75. 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.

76. 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.

77. T. Dudev, Y-l. 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.

78. 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.

79. R. Escribano, J.J. Sloan, N. Siddique, N. Sze and T. Dudev, "Raman Spectroscopy of Carbon-Containing Particles", *Vibr. Spectrosc.* **26** (2001) 179 – 186.

80. T. Dudev and C. Lim, "Modeling Zn^{2+}-Cysteinate Complexes in Proteins", *J. Phys. Chem. B* **105** (2001) 10709-10714.

81. S. Ilieva, B. Galabov, T. Dudev, T. Gounev and J.R. Durig, "Effective bond charges from infrared intensities in CH_4, SiH_4, GeH_4 and SnH_4", *J. Mol. Struct.* **565-566** (2001) 395 – 398.

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