

**PERSONAL INFORMATION**

- **Date of birth:** November, 12, 1968
- **Place of birth:** Almaty, Kazakhstan
- **Nationality:** Russian Federation
- **E-mail:** talgat.inerbaev@gmail.com; inerbayev\_tm@enu.kz
- **Web of Science ResearcherID:** AAB-7633-2020
- **ORCID:** 0000-0003-2378-4082

**AREAS OF SPECIALIZATION**

- Main fields - quantum chemistry, physical chemistry, materials science.
- Methods: density functional theory, density matrix theory, lattice and molecular dynamics.
- Current research interests: non-adiabatic charge relaxation in semiconductors; photocatalysis; chemical thermodynamics materials for energy applications; thermodynamics , kinetics and lattice dynamics of solids.

**EDUCATION**

- **Nikolaev Institute of Inorganic Chemistry**, Siberian Branch of Russian Academy of Science, Novosibirsk, Russia. Ph.D. in Chemical Physics, 2003. Theses: “*An influence of the guest molecules on the mechanical stability of the clathrate hydrates*”.
- **Nikolaev Institute of Inorganic Chemistry** Siberian Branch of Russian Academy of Science, Novosibirsk, Russia. M.S. in Physics, 1994. Theses: “*Spatial structural modulation induced by screened ferroelasticity*”.
- **Novosibirsk State University**, Novosibirsk, Russia. B.S. in Physics, 1992, Physics Department, Novosibirsk State University, Russia.

**EMPLOYMENT**

- May, 2012 – present: **L.N. Gumilyov Eurasian National University**, Astana, Kazakhstan  
Invited Professor at Physical&Technical Department
- November, 2009 – April, 2012: **South China Normal University**, Guangzhou, China  
Postdoctoral Research Associate at School of Chemistry and Environment
- February, 2008 – October, 2009: **University of Central Florida**, Orlando, FL, USA  
Postdoctoral Research Associate at NanoScience Technology Center
- December, 2003 – January, 2008: **Tohoku University**, Sendai, Japan  
Postdoctoral Research Associate at Institute for Materials Research
- September, 1994 – November, 2003: **Nikolaev Institute of Inorganic Chemistry**, Siberian Branch of Russian Academy of Science, Novosibirsk, Russia  
PhD student, Junior Researcher, Researcher

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## VISITING POSITIONS

- December 2008 - January 2009, Visiting Researcher, Institute for Materials Research, Tohoku University, Sendai, Japan
- October - December 2011, Visiting Researcher, Department of Material Sciences, Faculty of Engineering Sciences, Kyushu University, Fukuoka, Japan
- February 2012, Visiting Researcher, Institute for Materials Research, Tohoku University, Sendai, Japan
- July - August 2014, Visiting Researcher, Sobolev Institute of Geology and Mineralogy, Novosibirsk, Russia
- July 2016, Visiting Researcher, New Industry Creation Hatchry Center, Tohoku University, Sendai, Japan
- December 2016, Visiting Researcher, National University of Science and Technology MISIS, Moscow, Russian Federation
- July 2017, Visiting Researcher, New Industry Creation Hatchry Center, Tohoku University, Sendai, Japan
- August 2017, Visiting Researcher, National University of Science and Technology MISIS, Moscow, Russian Federation
- January 2018, Visiting Researcher, National Institute for Materials Science, Tsukuba, Japan
- August 2018, Visiting Researcher, New Industry Creation Hatchry Center, Tohoku University, Sendai, Japan
- January 2019, Visiting Researcher, National Institute for Materials Science, Tsukuba, Japan
- August 2019, Visiting Researcher, New Industry Creation Hatchry Center, Tohoku University, Sendai, Japan

## AWARDS AND EXTERNAL FUNDINGS

- **Grant of Ministry of Science and Education Republic of Kazakhstan** "First-principles design of perspective thermoelectric semiconductor materials" (15,000,000 KZT), 2018–2020 (PI).
- **Grant of Ministry of Science and Education Republic of Kazakhstan** "First principles design of effective magnetostriction materials for practical applications" (27,000,000 KZT), 2020–2022 (PI).
- **Grant of Institute for Materials Research, Tohoku University, Japan** 19G0503 "Ab initio simulation to design novel materials for magnetostriction applicable to electric power generation devices" 360 000 JPY (PI)
- **Grant of Ministry of Science and Education Republic of Kazakhstan** "Computer simulation of fluoride- and oxide-based optoelectronic materials doped with rare earth elements" (18,000,000 KZT), 2015–2017 (PI).
- **Grant of Ministry of Science and Education Republic of Kazakhstan** "Ab-initio study

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of electronic structure and stability of double alkaline - alkaline earth carbonates, as a perspective materials for laser optics" (9,000,000 KZT), 2015–2017 (Co-PI).

- **Japan Society for the Promotion of Science**, (JSPS) 20 months duration postdoctoral fellowship award, Grant No. P 04683, 2004.
- **Grant-in-Aid for JSPS postdoctoral fellows** (1,000,000 JPY), 2004 (PI).
- **Allocation Year 2009-2010 Startup/Production Award** "Ceria nanoparticles as a perspective material for biomedical applications", (600,000 hours on NERSC SuperComputer System), Office of Science of the U.S. Department of Energy, Contract No. DE-AC02-05CH11231 (PI).
- **China Postdoctoral Science Foundation**, Grant No. 20110490902, "Photo-Induces Dissipative Electron Dynamics in TiO<sub>2</sub> Nanorod Catalyzed with RuO<sub>2</sub>"(30,000 CNY), 2011 (PI).
- **Grant of Ministry of Science and Education Republic of Kazakhstan** N0. 556 on April, 27, 2013 "First Principles Modeling of Oxide Materials for Photocatalytic Water Splitting" (29,391,000 KZT), 2013–2015 (PI).
- **Grant of Ministry of Education and Science of the Russian Federation in the framework of the Increase Competitiveness Program of NUST MISIS** Modeling of non-equilibrium charge dynamics in semiconductors for solar energy conversion, Grant No. K3-2016-021 (800,000 Russian Roubles), 2016 (PI).
- **Grant of Ministry of Education and Science of the Russian Federation in the framework of the Increase Competitiveness Program of NUST MISIS** Computation-assisted understanding of high photovoltaic efficiency of lead trihalide perovskites, Grant No. K3-2017-026 (1,600,000 Russian Roubles), 2017 (PI).
- **Grant of Ministry of Education and Science of the Russian Federation in the framework of the Increase Competitiveness Program of NUST MISIS** First-principles design of perspective thermoelectric semiconductor materials, Grant No. K3-2018-022 (600,000 Russian Roubles), 2018 (PI).

**TEACHING EXPERIENCE**

**L.N.Gumilyov National University**

- Quantum Mechanics for undergraduate students
- Classical Electrodynamics for undergraduate students
- Computer Modeling of Physical Processes for master students
- Physics of Condensed Matter for master students
- Computational Materials Science for Ph.D. students
- Supervision of 10 Ph.D. students
- Supervision of 5 master students
- Supervision of 10 undergraduate students

**University of Central Florida**

- Co-supervision one graduate and two undergraduate students.

**Tohoku University**

- PhD Thesis co-supervision.

**Novosibirsk State University**

- Quantum Mechanics Computer Laboratories and Classical Mechanics classes Specialized Scientific Study Centre with a Physical-Mathematical and a Chemical-Biological Concentration, 1998–2003.
- Instructor of physics in Summer School in Specialized Scientific Study Centre with a Physical-Mathematical and a Chemical-Biological Concentration, 1993–1995.

## PUBLICATIONS

- **Papers (Web of Science):** 77
- **Non-ISI Journals Papers:** 4
- **Book Chapters:** 3
- **Conference Proceedings:** 11
- **Total Citation:** 1099 (Web of Science); 1261 (Scopus)
- **H-index:** 19 (Web of Science); 21 (Scopus)

## Papers

1. T. M. Inerbaev, Yu. Han, T. B. Bekker, D. S. Kilin "Mechanisms of Photoluminescence in Cu-Containing Fluoride Borate Crystals" *J. Phys.Chem.C*, accepted (IF=4.126)
2. F. Abuova, T. M. Inerbaev, A. Abuova, N.Merali, N. Soltanbek, G. Kaptagay, M. Sereдина, and V. Khovaylo "Structural, Electronic and Magnetic Properties of  $(\text{Mn})_2\text{Co}_{1-x}\text{V}_x\text{Z}$  (Z = Ga, Al) Heusler Alloys: An Insight from DFT Study" *Magnetochemistry*, 7 159 (2021) <https://doi.org/10.3390/magnetochemistry7120159> (IF=1.947)
3. T. M. Inerbaev, A. Abuova, Y. Kawazoe, R. Umetsu "Local ordering and interatomic bonding in magnetostrictive  $\text{Fe}_{0.85}\text{Ga}_{0.15}\text{X}$  (X=Ni,Cu,Co,La) alloy" *Computational Materials Science*, 202 110934 (2022) <https://doi.org/10.1016/j.commatsci.2021.110934> (IF=3.300)
4. K. Yusupov, T. Inerbaev, M. Rålander, D. Pankratova, I. Concina, A. J. Larsson, and A. Vomiero "Improved thermoelectric performance of Bi-deficient BiCuSeO material doped with Nb, Y, and P" *iScience*, 24, 103145 (2021). <https://doi.org/10.1016/j.isci.2021.103145> (IF=5.458)
5. T. B. Bekker, A. P. Yelisseyev, V. P. Solntsev, A. V. Davydov, T. M. Inerbaev, S. V. Rashchenko and A. I. Kostyukov "The influence of co-doping on the luminescence and thermoluminescence properties of Cu-containing fluoride borate crystals" *CrystEngComm*, 23, 6599–6609 (2021). <https://pubs.rsc.org/en/content/articlelanding/2021/CE/D1CE00556A> (IF= 3.545)
6. A. Ishteev, L. Luchnikov, D. S. Muratov, M.Voronova, A. Forde, T. Inerbaev, V. Vanyushin, D. Saranin, K. Yusupov, D. Kuznetsov,, Aldo Di Carlo "Single source chemical vapor deposition (ssCVD) for highly luminescent inorganic halide perovskite films" *Applied Physics Letters* 119, 071901 (2021) <https://doi.org/10.1063/5.0055993> (IF=3.791)
7. Fatima; T.M. Inerbaev, W. Xia, an D. Kilin "Magnetic-Field-Driven Electron Dynamics in Graphene" *Journal of Physical Chemistry Letters* 2021 , 12(19), 4749-4754 (IF=6.475)
8. N. Sagatov, A.-D.B. Bazarbek, T.M. Inerbaev, P.N. Gavryushkin, A.T. Akilbekov, K.D. Litasov "Phase Relations in the Ni-S System at High Pressures from *ab initio* Computations" *ACS Earth Space Chem.* 2021, 5(3), 596-603. (IF=3.475)

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9. K. Gima, T.M. Inerbaev, and D. Kilin "Excited state dynamics in a sodium and iodine co-doped lead telluride nanowire" *Molecular Physics*, 2021, 119(13), e1874557  
<https://doi.org/10.1080/00268976.2021.1874557> (Impact Factor = 1.837)
  10. N. Sagatov, P.N. Gavryushkin, I.V. Medrish, T.M. Inerbaev, K.D. Litasov "Phase Relations of Iron Carbides Fe<sub>2</sub>C, Fe<sub>3</sub>C, and Fe<sub>7</sub>C<sub>3</sub> at the Earth's Core Pressures and Temperatures" *Russian Geology and Geophysics* 2020, 61(12), 1345-1353.
  11. T.M. Inerbaev, N. Sagatov, D. Sagatova, P.N. Gavryushkin, A.T. Akilbekov, K.D. Litasov "Phase Stability in Nickel Phosphides at High Pressures" *ACS Earth Space Chem.* 2020, 4(11), 1978-1984. (IF=3.475)
  12. T.B. Bekker, T.M. Inerbaev, A.P. Yelisseyev, V.P. Solntsev, S.V. Rashchenko, A.V. Davydov, A.F. Shatskiy, and K.D. Litasov "Experimental and Ab Initio Studies of Intrinsic Defects in "Antizeolite" Borates with a Ba<sub>12</sub>(BO<sub>3</sub>)<sub>6</sub><sup>6+</sup> Framework and Their Influence on Properties" *Inorg. Chem.* 2020, 59(18), pp. 13598-13606 (IF=5.165)
  13. H. Pazniak, I.A. Plugin, M.J. Loes, T.M. Inerbaev, I.N. Burmistrov, M. Gorshenkov, J. Polcak, A.S. Varezchnikov, M. Sommer, D.V. Kuznetsov, M. Bruns, F.S. Fedorov, N.S. Vorobeva, A. Sinitskii, V.V. Sysoev, "Partially Oxidized Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXenes for Fast and Selective Detection of Organic Vapors at Part-per-Million Concentrations" *ACS Applied Nano Materials*, 3(4), pp. 3195-3204 (IF=5.097)
  14. A.U. Abuova, Yu.A. Mastrikov, E.A. Kotomin, S.N. Piskunov, T.M. Inerbaev, and A.T. Akilbekov "First-Principles Modeling of Oxygen Adsorption on Ag-Doped LaMnO<sub>3</sub> (001) Surface" *J. Electron. Mater.* 2020 49(2), pp. 1421-1434
  15. A. Forde, T.M. Inerbaev, and D. Kilin "Spectral Signatures of Positive and Negative Polarons in Lead-Halide Perovskite Nanocrystals" *J. Phys. Chem. C* 2020 Vol. 124(1), pp. 1027-1041 (IF=4.126)
  16. G.A. Kaptagay, T.M. Inerbaev, A.T. Akilbekov, N.O. Koilyk, A.U. Abuova, N.A. Sandibaeva, "First principles modelling of the N-doped Co<sub>0.5</sub>-terminated (001) Co<sub>3</sub>O<sub>4</sub> surface" *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* 2020 Vol. 465 pp. 11-14
  17. A. I. Voronin, I. A. Serhienko, Ye. Zh. Ashim, V. L. Kurichenko, A. P. Novitskii, T.M. Inerbaev, R. Umetsu, and V. V. Khovaylo "Electrical Transport Properties of Nb and Ga Double Substituted Fe<sub>2</sub>VAl Heusler Compounds" *Semiconductors*, 2019, Vol. 53, No. 13, pp. 1856-1859.
  18. Sagatov, N.E., Gavryushkin, P.N., Banayev, M.V., T.M. Inerbaev, Litasov, K.D. "Phase relations in the Fe-P system at high pressures and temperatures from ab initio computations" *High Pressure Research* 2020, 40(2), pp. 235-244

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19. T.M. Inerbaev, Forde, A., Jensen, S.J., Kilin, D "Spin-Unrestricted and Spinor Nonradiative Relaxation Dynamics in Functionalized Semiconductors" ACS Symposium Series, 2019 Vol. 1331, pp. 1-22
  20. Ye. Zh. Ashim, T.M. Inerbaev, A.T. Akilbekov, H. Miki, T.Takagi, and V.V. Khovaylo "Theoretical Modeling of the Thermoelectric Properties of  $\text{Fe}_2\text{Ti}_{1-x}\text{V}_x\text{Sn}$  Heusler Alloys" *Semiconductors*, **2019** 53(7), pp. 879-882.
  21. Litasov K.D., Inerbaev T.M., Abuova, F.U., Chanyshv A.D., Dauletbekova A.K., Akilbekov A.T., "Elastic properties of polycyclic aromatic hydrocarbons at high pressures from first principles calculations", *Geochemistry International*, **2019** 57 (5), pp. 499-508 (Impact Factor = 0.699)
  22. Fatima, Y. Han, D.J. Vogel, T.M. Inerbaev, N.Oncel, E. K. Hobbie, and D. S. Kilin "Photoexcited Electron Lifetimes Influenced by Momentum Dispersion in Silicon Nanowires" *Journal of Physical Chemistry C* **2019**, 123(12), pp 7457-7466 (Impact Factor = 4.772)
  23. A. Forde, T.M. Inerbaev, E. Hobbie, and D.S. Kilin "Excited-State Dynamics of a  $\text{CsPbBr}_3$  Nanocrystal Terminated with Binary Ligands: Sparse Density of States with Giant Spin-Orbit Coupling Suppresses Carrier Cooling" *Journal of the American Chemical Society* **2019**, 141(10), pp 4388-4397 (Impact Factor = 14.357)
  24. A.I.Voronin, A.P.Novitskii, Y.Z.Ashim, T.M. Inerbaev, N.Yu.Tabachkova, V.T.Bublik, V.V.Khovaylo "Exploring the origin of contacts destruction in tetradymite-based thermoelectric elements" *Journal of Electronic Materials* **2019** 48(4), pp 1932-1938 (Impact Factor = 1.566)
  25. N. Sagatov, P.N. Gavryushkin, T.M. Inerbaev and K.D. Litasov "New high-pressure phases of  $\text{Fe}_7\text{N}_3$  and  $\text{Fe}_7\text{C}_3$  stable at Earth's core conditions: evidences for carbon-nitrogen isomorphism in Fe-compounds" *RSC Adv.*, **2019**, 9, 3577-3581 (Impact Factor = 2.936)
  26. Fatima, J. Vogel, T.M. Inerbaev, N. Oncel, and D. Kilin "First-Principles Study of Electron Dynamics with Explicit Treatment of Momentum Dispersion on Si Nanowires along Different Directions" *Molecular Physics* DOI:10.1080/00268976.2018.1538624 (Impact Factor = 1.837)
  27. A. Forde, T.M. Inerbaev, D. S. Kilin "Spinor Dynamics in Pristine and  $\text{Mn}^{2+}$  Doped  $\text{CsPbBr}_3$  NC: Role of Spin-Orbit Coupling in Ground and Excited State Dynamics" *Journal of Physical Chemistry C* **2018** 122(45) 26196-26213 (Impact Factor = 4.772)
  28. Fatima, J. Vogel, T.M. Inerbaev, N. Oncel, and D. Kilin "First-Principles Study of Charge Carrier Dynamics with Explicit Treatment of Momentum Dispersion on Si Nanowires along  $\langle 211 \rangle$  crystallographic Directions" *MRS Advances* **2018** 3(59) 3477-3261
  29. A. Forde, T.M. Inerbaev, D. S. Kilin "Role of Cation-Anion Organic Ligands for Optical Properties of Fully Inorganic Perovskite Quantum Dots" *MRS Advances* **2018** 3(59) 3255-3261

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30. P.N. Gavryushkin, N. Sagatov, Z.I. Popov, A. Bekhtenova, T.M. Inerbaev, K.D. Litasov "Structure and Properties of Novel High-Pressure Phases of Fe<sub>7</sub>N<sub>3</sub>" *JETP Letters* **2018** 107 389-393 (Impact Factor = 1.235)
  31. D. J. Vogel, T.M. Inerbaev, D. S. Kilin "Role of Lead Vacancies for Optoelectronic Properties of Lead-Halide Perovskites" *Journal of Physical Chemistry C* **2018** 122 5216-5226 (Impact Factor = 4.772)
  32. Y. Han, D.J. Vogel, T.M. Inerbaev, P.S. May, M.T. Berry, D.S. Kilin "Photoinduced Dynamics to Photoluminescence in Ln<sup>3+</sup> (Ln = Ce, Pr) Doped  $\beta$ -NaYF<sub>4</sub> Nanocrystals Computed in Basis of Non-Collinear DFT with Spin-Orbit Coupling" *Molecular Physics* **2018** 116 697-707 (Impact Factor=1.837) (Impact Factor=1.837)
  33. P N. Gavryushkin, N.S. Martirosyan, T.M. Inerbaev, Z.I.Popov, S.V. Rashchenko, A.Yu. Likhacheva, S.S. Lobanov, A.F. Goncharov, V.B. Prakapenka, and K.D. Litasov "Aragonite-II and CaCO<sub>3</sub>-VII - New High-Pressure High-Temperature Polymorphs of CaCO<sub>3</sub>", *Crystal Growth&Design*, **2017**, 17(12) 6291-6296 (Impact Factor = 4.055)
  34. S.J. Jensen, T.M. Inerbaev, A.U. Abuova, D.S. Kilin, "Spin Unrestricted Nonradiative Relaxation Dynamics of Cobalt-Doped Anatase Nanowire" *Journal of Physical Chemistry C* **2017**, 121 (30) 16110-16125. (Impact Factor = 4.772)
  35. D.J. Vogel, A. Kryjevski, T.M. Inerbaev, D.S. Kilin "Photoinduced Single- and Multiple-Electron Dynamics Processes Enhanced by Quantum Confinement in Lead Halide Perovskite Quantum Dots" *Journal of Physical Chemistry Letters* **2017**, 120 (33) 18909-18916. (Impact Factor = 9.542)
  36. K.D. Litasov, A. Shatskiy, P.N. Gavryushkin, A.E. Bekhtenova, P.I. Dorogokupets, B.S. Danilov, Y. Higo, A.T. Akilbekov, T.M. Inerbaev "*P-V-T* equation of state of CaCO<sub>3</sub> aragonite to 29 GPa and 1673 K: In situ X-ray diffraction study" *Physics of the Earth and Planetary Interiors* **2017**, 265 82-91 (Impact Factor = 2.319)
  37. T.M. Inerbaev, A. Dauletbekova, A. Abdrakhmetova "Irradiation effect on infrared spectra of LiF:OH crystals: Theoretical modeling" *Physica B* **2017** 521 258-263 (Impact Factor = 1.386)
  38. S.L. Brown, D.J. Vogel, J.B. Miller, T.M. Inerbaev, R.J. Anthony, U.R. Kortshagen, D.S. Kilin, and E.K. Hobbie "Enhancing Silicon Nanocrystal Photoluminescence through Temperature and Microstructure" *Journal of Physical Chemistry C* **2016**, 120 (33) 18909-18916. (Impact Factor = 4.772)
  39. S. J. Jensen, T.M. Inerbaev, D. S. Kilin "Spin Unrestricted Excited State Relaxation study of Vanadium (IV) Doped Anatase" *Journal of Physical Chemistry C* **2016** 120(11) 5890-5905. (Impact Factor = 4.772)



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40. G.A. Kaptagay, T.M. Inerbaev, Yu.A. Mastrikov, E.A. Kotomin, A.T. Akilbekov "Water interaction with perfect and fluorine-doped  $\text{Co}_3\text{O}_4$  (100) surface" *Solid State Ionics* **2015** 277 77–82. (Impact Factor = 2.112)
  41. A.U. Abuova, Yu.A. Mastrikov, E.A. Kotomin, Y. Kawazoe, T.M. Inerbaev, A.T. Akilbekov "First principles modeling of Ag adsorption on the  $\text{LaMnO}_3$  (001) surfaces" *Solid State Ionics* **2015** 273 46–50. (Impact Factor = 2.112)
  42. K. D. Litasov, P. N. Gavryushkin, A. S. Yunoshev, S. V. Rashchenko, T.M. Inerbaev, and A. T. Akilbekov "Thermal expansion of coronene  $\text{C}_{24}\text{H}_{12}$  at 185–416 K" *Journal of Thermal Analysis and Calorimetry* **2015** 119 1183-1189 (Impact Factor = 2.206)
  43. T.M. Inerbaev, A. S. Karakoti, S. V. N. T. Kuchibhatla, A. Kumar, A. E. Masunov, and S. Seal "Aqueous medium induced optical transitions in cerium oxide nanoparticles" *Physical Chemistry Chemical Physics* **2015** 17 6217–6221 (Impact Factor = 4.772)
  44. S. Huang, T. M. Inerbaev, D. S. Kilin "Excited State Dynamics of  $\text{Ru}_{10}$  Cluster Interfacing Anatase  $\text{TiO}_2$  (101) Surface and Liquid Water" *Journal of Physical Chemistry Letters* **2014** 5 2823–2829 (Impact Factor = 9.542)
  45. A. Likhacheva, S. Rashchenko, A. Chanyshv, T. M. Inerbaev, K. Litasov, and D. Kilin "Thermal Equation of State of Solid Naphthalene to 13 GPa and 773 K: In Situ X-ray Diffraction Study and First Principles Calculations" *Journal of Chemical Physics* **140**, 164508 (2014) (Impact Factor = 3.164)
  46. J. Chen, A. Schmitz, T. Inerbaev, Q. Meng, S. Kilina, S. Tretiak, and Dmitri S. Kilin "First-Principles Study of p-n-Doped Silicon Quantum Dots: Charge Transfer, Energy Dissipation, and Time-Resolved Emission" *Journal of Physical Chemistry Letters* (2013) **4**, 2906–2913, (Impact Factor = 9.542)
  47. J. D. Gaynor, A. S. Karakoti, T. Inerbaev, S. Sanghavi, P. Nachimuthu, V. Shutthanandan, S. Seal, and S. Thevuthasan "Enzyme-free Detection of Hydrogen Peroxide from Cerium Oxide Nanoparticles Immobilized on Poly(4-vinylpyridine) SAMs" *Journal of Materials Chemistry B* (2013) **1** 3443–3450 (Impact Factor = 5.968)
  48. Inerbaev T., Hoefelmeyer J., and Kilin D., "Photoinduced charge transfer from titania to surface doping site" *Journal of Physical Chemistry C* (2013) **117** 9673–9692 (Impact Factor = 4.772)
  49. K. Liu, T. M. Inerbaev, J. Korchowiec, and F. L. Gu, and Y. Aoki, "Geometry optimization for large systems by the elongation method", *Theoretical Chemistry Accounts*, (2012) 131:1277 (Impact Factor = 2.903)
  50. L. Z. Kang, T. M. Inerbaev, B. Kirtman, and F. L. Gu "Alkali metal doping effect on static first hyperpolarizabilities of PMI chains", *Theoretical Chemistry Accounts* **130** 727–737 (2011). (Impact Factor = 2.903)

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51. T. M. Inerbaev, F. L. Gu, H. Mizuseki and Y. Kawazoe "Theoretical Study of Solvent Effect on the Structure, First Electronic Excited State and Nonlinear Optical Properties of Substituted Stilbazolium Cations", *International Journal of Quantum Chemistry* **111** 780 – 787 (2011). (Impact Factor = 1.302)
  52. S. Ganopadhyay, A. E. Masunov, T. Inerbaev, J. Mesit, R. K. Guha, A. K. Sleiti, J. S. Kapat, "Understanding oxygen vacancy migration and clustering in barium strontium cobalt iron oxide", *Solid State Ionics* **181** 1067 – 1073 (2010). (Impact Factor = 2.741)
  53. T. M. Inerbaev, S. Seal and A.E. Masunov "Density functional study of oxygen vacancy formation and spin density distribution in octahedral ceria nanoparticles", *Journal of Molecular Modeling* **16** 1617 – 1623 (2010). (Impact Factor = 2.336).
  54. T. M. Inerbaev, Y. Kawazoe and S. Seal, "Theoretical Calculations of Hydrogen Adsorption by SnO<sub>2</sub> (110) Surface: Effect of Doping and Calcination", *Journal of Applied Physics* **107** 104504 (2010). (Impact Factor = 2.072).
  55. A. Vincent, T. M. Inerbaev, S. Babu, A.S. Karakoti, W.T. Self, A.E. Masunov and S. Seal, "Tuning Hydrated Nanoceria Surfaces: Experimental/Theoretical Investigations of Ion Exchange and Implications in Organic and Inorganic Interactions", *Langmuir* **26** 7188 – 7198 (2010). (Impact Factor = 4.269).
  56. T. M. Inerbaev, R. Sahara, H. Mizuseki, Y. Kawazoe, and T. Nakamura, "Reducible and non-reducible defect clusters in tin-doped indium oxide", *Solid State Communications* **150** 18 – 21 (2010) (Impact Factor = 1.979).
  57. T. Inerbaev, A. E. Masunov, S. I. Khondaker, A. Dobrinescu, A.-V. Plamadà, Y. Kawazoe, "Quantum Chemistry of Quantum Dots: Effects of Ligands and Oxidation", *Journal of Chemical Physics*, **131** 044106 (2009). (Impact Factor = 3.093).
  58. S. Gangopadhyay, T. Inerbaev, A. E. Masunov, N. Orlovskaya, "Structural Characterization combined with the First Principles Simulations of Barium/ Strontium Ferrate/Cobaltate as a Promising Material for SOFC", *ACS Applied Materials & Interfaces*, **1** 1512 – 1519 (2009). (Impact Factor = 6.723).
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