Xuanhao Chang

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#### EDUCATION

Lomonosov Moscow State University

Ph.D. in Physical Chemistry; Department of Chemistry

 $Vibrational - rotational \ Molecular \ spectroscopy, \ Computational \ spectroscopy.$ 

National Research Tomsk Polytechnic University
Master of Physics; Research School of High-Energy Physics

High-resolution vibrational-rotational spectroscopy.

National Research Tomsk State University

Academic Mobility; Faculty of Physics Theoritical Physics.

National Research Tomsk Polytechnic University

Bachelor of Physics; Research School of High-Energy Physics

Jilin University

Bachelor of Physics; College of Physics

Tomsk, Russia

Moscow, Russia

Tomsk. Russia

Sep 2019 - Sep 2023

Sep 2017 - Jul 2019

Sep 2016 - Jul 2018

Tomsk, Russia Aug 2015 - Jul 2017

Changchun, China

Aug 2013 - Aug 2015

# SKILLS SUMMARY

• Languages: Chinese(Native), Russian(Advanced), English(Good skills)

- Programming: Wolfram Mathematica, Fortran77/95/08 (OpenMP and Coarray), Latex, Python
- Tools: Visual Studio Community/Code, Gaussian, Cfour, Origin, Windows/Lunix
- Knowledge and Interests: Quantum Chemistry, Molecular ro-vibrational spectroscopy, Perturbation theory, Lie group/algebra,
   Differential geometry, Irreducible tensorial operator

# AWARDS AND FELLOWSHIPS

• Chinese Scholarship Council Fellowship, 2015-2023

# EXPERIENCE

### The laboratory of quantum chemistry and molecular modeling

Software Developer

Moscow, Russia

Sep 2019 - July 2023

- ANCO program developing: Theory and software design, debugging by comparison with Wolfram Mathematica
- RSPT, RSPT\_L, PADE programs developing: Development in theory, debugging and analyzing

# Department of Chemistry, Lomonosov Moscow State University

Teaching Assistant - Prof. Uspenskaya I.A.

Moscow, Russia

Jan 2021 - Dec 2021

o Physical Chemistry, Part I,II: Leading weekly seminar and colloquiums

Department of Chemistry, Lomonosov Moscow State University

Teaching Assistant - Prof. Novakovskaya Yu.V.

Moscow, Russia

Sep 2020 - Dec 2020

 $\circ~{\bf Quantum~Chemistry~and~Molecular~structure}.$  Leading weekly seminar

# Publications

- (2023) <u>Xuanhao C.</u>, Dobrolyubov E. O., Krasnoshchekov S. V.,: Normal Ordering of the Angular Momentum Cylindrical Ladder Operators and their Products with Wigner  $D_{0,\varepsilon}^1$  functions. (To be submitted)
- (2023) <u>Xuanhao C.</u>, Krasnoshchekov S. V.,: Ab initio line lists and Watson A reduction effective Hamiltonians predicted by the Van Vleck canonical operator perturbation theory. (Under Review)
- (2023) <u>Xuanhao C.</u>, Dobrolyubov E. O., Krasnoshchekov S. V., Spectrochim. Acta A, 122071: Vibrational resonance analysis of linear molecules using resummation of divergent rayleigh—schrödinger perturbation theory series. DOI: 10.1016/j.saa.2022.122071
- (2022) <u>Xuanhao C.</u>, Dobrolyubov E. O., Krasnoshchekov S. V., Phys. Chem. Chem. Phys., 24(11), p.6655-6675: Fundamental studies of vibrational resonance phenomena by multivalued resummation of divergent Rayleigh-Schrödinger perturbation theory series: deciphering polyad structures of three  $H_2$  <sup>16</sup>O isotopologues. DOI: 10.1039/d1cp04279c

- (2021) Krasnoshchekov S. V., Egor O. D., <u>Xuanhao C.</u>, JQSRT, 268, 107620: Hypoflorous acid (hof): A molecule with a rare (1,-2,-1) vibrational resonance and (8,3,2) polyad structure revealed by padé-hermite resummation of divergent rayleigh-schrödinger perturbation theory series.

  DOI: 10.1016/j.jqsrt.2021.107620
- (2020) Krasnoshchekov S. V., Egor O. D., Xuanhao C., Optics and Spectroscopy, 128(12), p.1927-1938: Fundamental Analysis of Singular and Resonance Phenomena in Vibrational Polyads of the Difluorosilylene Molecule. DOI: 10.1134/S0030400X20120942
- (2020) <u>Xuanhao C.</u>, Krasnoshchekov S. V., Pupyshev V. I., Millionshchikov D. V., Phys. Lett. A, 384(19), 126493: Normal ordering of the su(1, 1) ladder operators for the quasi-number states of the Morse oscillator. DOI: 10.1016/j.physleta.2020.126493
- (2019) Krasnoshchekov S. V., <u>Xuanhao C.</u>, Int. Rev. Phys. Chem., 38(1), p.63-113: Ladder operators for Morse oscillator and a perturbed vibrational problem. DOI: 10.1080/0144235X.2019.1593583
- (2018) S. Chan, O. V. Gromova, E. S. Bekhtereva, C. Leroy, O. N. Ulenikov, Russian Physics Journal, 61, p.516–520: Determination of Irreducible Rotational operators on the rotation SO(3) group and  $T_d$  point symmetry. DOI: 10.1007/s11182-018-1428-0

#### Presentations in International Conferences

- (2023) <u>Xuanhao C.</u>, Krasnoshchekov S. V.,: "Ab Initio Solution of the Vibration-Rotation Problem with Watson Hamiltonian by Van Vleck Operator Perturbation Theory", The 26th International Conference on High Resolution Molecular Spectroscopy (PRAHA2022, Aug 29th Sep 2nd, 2022), oral presentation
- (2023) <u>Xuanhao C.</u>, <u>Dobrolyubov E. O.</u>, <u>Krasnoshchekov S. V.</u>,: "Vibrational resonance analysis of acetylene using the large order perturbation series and Pade-Hermite approximant", The 26th International Conference on High Resolution Molecular Spectroscopy (PRAHA2022, Aug 29th Sep 2nd, 2022), **Poster**
- (2023) Dobrolyubov E. O., <u>Xuanhao C.</u>, Krasnoshchekov S. V.,: "Resonance and Polyads of Carbonyl Sulphide (OCS) Isotopologues Studied by Padé-Hermite Resummation of Divergent RSPT Series", The 26th International Conference on High Resolution Molecular Spectroscopy (PRAHA2022, Aug 29th Sep 2nd, 2022), **Poster**
- (2019) Chang X., Krasnoshchekov S. V., Bekhtereva E.S.: "Ladder Operators for the Morse Oscillator and their application for a perturbed vibrational problem", The 26th Colloquium on High Resolution Molecular Spectroscopy (HRMS Dijon 2019, Aug 26-30, 2019), Poster