Academic Positions

2021-current **Post-doctoral researcher,** Department of Chemistry, University of Wisconsin-Madison (Advisor: Prof. Xuhui Huang)

Current projects:

- A study of mutations that underlie cancer and intellectual disability in protein phosphatase 2A that disrupt normal autoinhibition via allosteric pathways
- A study of the interplay between chaperone Hsp70 and the folding of client proteins
- Simulations of terminal alkyne-modified DNA aptamers with enhanced protein binding affinity

Work experience

2017 **Web application designer**, Mitotech Pharma, Moscow, Russia

I designed and integrated graphical web applications for bioinformatics research projects. My results are part of the following publications:

- Klimchuk, O. I., Konovalov, K. A., Perekhvatov, V. V., Skulachev, K. V., Dibrova, D. V., & Mulkidjanian, A. Y. (2017). COGNAT: a web server for comparative analysis of genomic neighborhoods. Biology direct, 12(1), 1-7.
- Dibrova, D. V., Konovalov, K. A., Perekhvatov, V. V., Skulachev, K. V., & Mulkidjanian, A. Y. (2017). COGcollator: a web server for analysis of distant relationships between homologous protein families. Biology direct, 12(1), 1-11.

Education

2017-2021 **Ph.D. in Chemistry**, Department of Chemistry, Hong Kong University of Science and Technology, Hong Kong (Advisor: Prof. Xuhui Huang)

- Thesis: "Mechanisms of Transcription: RNA Polymerase II Elongation Complex with DNA Modifications Studied with Molecular Dynamics Simulations*" (In silico* study of RNA polymerase II transcription with DNA modifications, using molecular dynamics simulations and Markov state models.)

2011-2017 **Specialist in Fundamental and Applied Chemistry**, Lomonosov Moscow State University, Department of Chemistry, Russia, with honors, (Advisor: Prof. Andrey Golovin)

- Thesis: "A study of phosphonate-hydrolyzing antibodies" (*In silico* design of phosphonate hydrolyzing abzymes, employing molecular dynamics simulations, metadynamics, QM/MM simulations and protein structure modeling.)

Professional Skills

- Primary skills: conducting and analyzing molecular dynamics simulations with atomistic and coarse-grained models, Markov state models, enhanced sampling methods (e.g., metadynamics, REST), *in silico* protein design (Rosetta), QM/MM simulations
- Coding: Python, R, Java, jQuery, Angular, C/C++

Primary Publications

1. **Konovalov, K.A.,** Unarta, I.S., Cao, S., Goonetilleke1, E.C., Huang, X.*, "Markov state models to study the functional dynamics of proteins in the wake of machine learning", *J. Am. Chem. Soc. Au*, 1(9), 1330-1341, (2021)
2. **Konovalov, K. A.,** Wang, W., Wang, G., Goonetilleke, E. C., Gao, X., Wang, D., & Huang, X. A comprehensive mechanism for 5-carboxylcytosine-induced transcriptional pausing revealed by Markov state models. *Journal of Biological Chemistry*, 296, (2021)
3. **Konovalov, K.A.**, Pardo-Avila, F., Tse, C.K.M., Oh, J., Wang, D., Huang, X., 8-oxo-guanine DNA damage induces transcription errors by escaping two distinct fidelity control checkpoints of RNA polymerase II, *Journal of Biological Chemistry*, (2019)

Fellowships and Awards

1. 2017-2021, Hong Kong Ph.D. fellowship scheme (Hong Kong)
2. Scientific debate competitions:
   - 2015 1st prize, Tournament of Three Sciences (Voronezh, Russia)
   - 2015 2nd prize, Students tournament of Natural Sciences (Minsk, Belarus)
   - 2014 3rd prize, Biotournament (Puschino, Russia)

Teaching Experience

2017-2019 Teaching assistant, HKUST, Hong Kong

- Laboratory for General Chemistry I (CHEM1050)
- Physical Chemistry Laboratory (CHEM2450)
- Molecular Characterization Laboratory (CHEM3555)
- Mathematical Methods in Physical Chemistry (CHEM 2409)

2023 Course coordinator, UW Madison, WI

- Graduate Studen Seminar (CHEM960)