Kirill A. Konovalov

mail: konovalov@wisc.edu
mail2: kirillkirill0@gmail.com
Department of Chemistry
University of Wisconsin-Madison

I specialize in studying complex protein and nucleic acid dynamics through computer simulations. My aptitude lies with physical chemistry, particularly, biophysical models based on methods ranging from quantum mechanics to residue-level coarse-grained, with a focus on Markov state models and enhanced sampling. Overall, my work has contributed to our understanding of biophysics, specifically, transcription with RNA polymerase II and antibody design.

Academic Positions

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

Current projects:

- A computational study of the allosteric effect of mutations in Protein Phosphatase 2A that underlie cancer and intellectual disability
- A computational study of the interplay between chaperone Hsp70 and the folding of client proteins

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

Google scholar

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 between teams:
   - 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)