

Jing Yang

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EDUCATION

- 09/2015–Present Graduate Student: Science Education, Department of Curriculum and Instruction
School of Education, Indiana University, Bloomington, IN
Advisor: Prof. Adam Maltese
- 09/2011–Present PhD candidate: Physical and Theoretical Chemistry, Department of Chemistry
School of Arts and Sciences, Indiana University, Bloomington, IN
Advisor: Prof. Peter J. Ortoleva
- 09/2006-07/2010 B.S. College of Chemistry, Beijing Normal University, China
Major: Chemistry
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PROFESSIONAL EXPERIENCE

Fall 2011-Present Indiana University Bloomington – Associate Instructor
C103: Introduction to Chemical Principles
C117: Principles of Chemistry and Biochemistry I
C127: Principles of Chemistry and Biochemistry I Lab

Summer 2014&2015 The Foundations in Science and Mathematics (FSM) summer program – Instructor
FSM is a graduate student led initiative designed to help local high school students prepare for their upcoming math and science courses. I was responsible for Chemistry I course development and teaching in 2014. I'll involve into grant writing, registration, and new chemistry course developing.

10/2007–12/2007 Beijing Bayi Middle School – Instructor
I was responsible for course development and teaching for the Astronomy Team about basic astronomy knowledge, usage of telescopes, and directing their observation.

Others: guide visiting undergraduates and high school students in Prof. Ortoleva's group.

PUBLICATIONS

Refereed Journal Articles

J. Grosch, **J. Yang**, A. Shen, Y.V. Sereda, and P.J. Ortoleva, Broad Spectrum Assessment of the Epitope Fluctuation - Immunogenicity Hypothesis, Vaccine, in press, 2015

A. Abi-Mansour, Y.V. Sereda, **J. Yang**, and P.J. Ortoleva Prospective on Multiscale Simulation of Virus-like Particles: Application to Computer-aided Vaccine Design, *Vaccine*, in press, 2015

J. Jiang, **J. Yang**, Y.V. Sereda and P.J. Ortoleva, Early Stage P22 Viral Capsid Self-Assembly Mediated by Scaffolding Protein: Atom-Resolved Model and Molecular Dynamics Simulation, *the Journal of Physical Chemistry B* (2015) 19 (16), pp 5156–5162

J. Yang, A. Singharoy, Y.V. Sereda and P.J. Ortoleva, Quasiequivalence of Multiscale Coevolution and Ensemble MD Simulations: A Demonstration with Lactoferrin, *Chemical Physics Letters* (2014) pp. 154-160

Y. Huang, **J. Yang**, K. Zhao, A Method for Detecting Sugar Content in Alcoholic Beverages by Dielectric Spectroscopy, *Food Science* (in Chinese), (2013) 35: 149-154

J. Zhao, K. Jiao, **J. Yang**, C. He, and H. Wang, Mechanically Strong and Thermosensitive Macromolecular Microsphere Composite Poly(N-isopropylacrylamide) Hydrogels, *Polymer*, 54(6):1596-1602 (2013).

K. Wang, T. Su, **J. Yang**, H. Zhang, W. Sun, A Comprehensive Design to Improve Undergraduate Chemistry Experiment-Toluene as a Solvent to Silanize the Glass Subsurface Instead of Ethanol During the Process to Prepare Electrostatic Self-Assemble Film, *Chinese Journal of Chemical Education*, 7:64-65 (2009).

Conferences

J. Yang, J.M. Espinosa-Duran, A. Abi Mansour and P. Ortoleva (2013, September), Reaction-mediated Structural Transitions in Supramolecular Assemblies: Multiscale Methods and Demonstration for a Virus-like Particle, 246th ACS National Meeting & Exposition (selected to participate the NVIDIA Award competition)

K. Jiao, **J. Yang**, J. Zhao and H. Wang (2009, July), Macromolecular Microsphere Composite Poly(N-Isopropylacrylamide) Hydrogel with High Mechanical Strength and Thermo-sensitivity With Pre-Irradiation Method, Chinese Annual Macromolecule Meeting

Manuscripts in preparation

J. Yang, A. Abi Mansour, and P.J. Ortoleva, Multiscale Factorization of Chemically Transforming Nanosystems: coupled structure –Reaction Dynamics in VLPs

J. Yang, and P.J. Ortoleva, Multiscale Theory of Nanoreactors: The Michaels-Menton Kinetics

J. Yang, and P.J. Ortoleva, Relation of three multiscale methods for simulating classical many-particle systems

J. Jiang, **J. Yang**, J.M. Espinosa-Duran, and P. Ortoleva, All-atom Molecular Dynamics Simulations of Bacteriophage P22 Capsid Suggest Insights on Temperature Induced Viral Structural Transition

RESEARCH

Projects in Science Education:

Interested in improving Undergraduate STEM education.

Projects in Chemistry:

Equivalence of Multiscale Modeling and Ensemble MD

The microstate (i.e., the atomic positions and momenta) and CG states coevolve via a strongly coupled

dynamic that gives these systems a fundamentally multiscale character. With this, all-atom MD simulations can be achieved with great efficiency. The goal of this project is to demonstrate that our multiscale approach and ensemble MD simulation methods generate identical results.

Multiscaling for Coupled Reaction-structure Model

Reactions typically are rare events when compared to the timescale of atomic vibrations. The multiscale timestepping provides a convenient platform for simulating the coupled reaction-structure kinetics. A coupled reaction-structure method is developed for addressing rare reaction events in P22 in a way that accounts for the rate of traversal of the capsule, and effects such as molecular crowding and migration of reactants and products within the interior.

Vaccine Discovery: A Computer-Aided Approach

A VLP-based strategy has proven successful in developing highly effective and safe vaccines against infectious diseases. By integrating advanced nanoparticle simulation, bioinformatics, standard nanoparticle synthesis methods, and traditional laboratory immunogenicity testing, we achieve a highly efficient workflow for vaccine computer-aided discovery.

Others Projects:

Undergraduate Graduation Project (12/2009-07/2010): Assessment of Frying Oil Quality with Dielectric Spectroscopy

Comprehensive Experiment Design (10/2008): Preparation of Self-Assembled Film

Undergraduate Scientific Research (04/2008-08/2009): Thermo-sensitive Hydrogels with High Mechanical Strength

AWARDS

2013 Provost Travel Award to 246th ACS National Meeting & Exposition