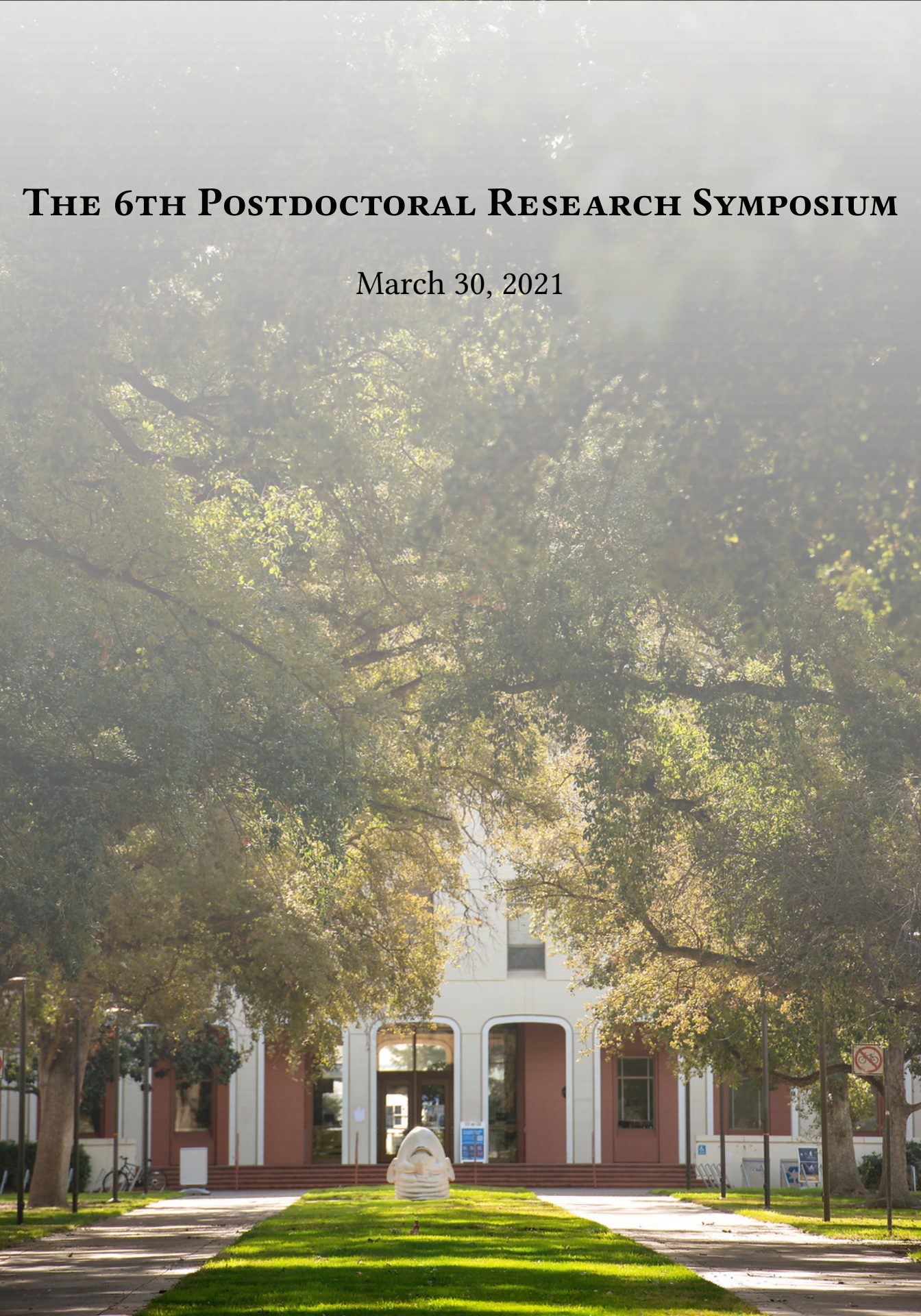


THE 6TH POSTDOCTORAL RESEARCH SYMPOSIUM

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ACTIVE INFERANTS: AN ACTIVE INFERENCE MODEL FOR ANT COLONY BEHAVIOR

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Ant colonies are distributed entities that engage in effective collective action despite fundamental nestmate-level uncertainty. Because of their ecological diversity and algorithmic ingenuity, studies of ant colony behavior have provided insight into areas such as logistics, construction, information flow, and optimization. In this research, we introduce a model of ant colony foraging behavior that uses the framework of Active Inference (an action-oriented theory related to the Free Energy Principle). We use a Python simulation to implement and visualize a model of ant colony foraging behavior. We characterize some of the emergent dynamics of the simulation and lay out avenues for future simulations and work in robotics, ecology, neuroscience, and philosophy.

DNA PHOTOLYASE: MOLECULAR MACHINERY FOR REPAIR OF UV-INDUCED DAMAGE IN DNA

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*Joint work with Alexei Stuchebrukhov. Contribution of UC Davis, USA and IChTM, University of Belgrade, Serbia.

Damages in DNA structure are often caused by UV light, ionizing radiation, toxic substances and environmental pollution. To maintain genetic stability, cells protect themselves against these kinds of lesions. Moreover, the main DNA repair processes in prokaryotic and eukaryotic cells are quite similar. Photolyases repair the major DNA defects—cyclobutane pyrimidine dimers (CPD) and (6-4)-photoproducts. The enzyme contains two photoactive cofactors: folate—the photon antenna molecule and catalytically active FADH—form. Photolyase repairs UV (200-300 nm) induced damage in DNA by splitting the ring of CPD dimer into pyrimidine monomers. If not repaired the CPD lesions are highly cytotoxic, mutagenic, and carcinogenic.

In the present theoretical/computational study of photolyase from *E. coli*, continuum electrostatic and electron tunneling currents methods are employed to get a full insight into photoactivation and photorepair mechanism of the enzyme and the structure-function interrelation. Protonation state of titratable residues, redox potentials of the conserved tryptophan triad, the energetics and kinetic reaction rates are calculated comparing well with available experimental data. The free energies of all potentially relevant enzyme states during the photoreactivation mechanism are evaluated.

This presentation also addresses a several long-time controversial questions about the biological relevance of unusual U-shape of FADH cofactor; hopping vs. super-exchange mechanism of the ET pathway; the shortest FADH⁻ to CPD distance, after flipping out the CPD damage to the active site, in the CPD-protein complex or presence of radical FADH^{*} state in the resting state of photolyase. The study could be relevant for other types of photolyases and cryptochromes, which all share the same structural features.

NEW INSIGHTS INTO THE MULTI-OMICS PREDICTION GAINED FROM OAT BREEDING POPULATIONS

Haixiao Hu

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The multi-omics prediction has been shown superior to genomic prediction for predicting phenotypes. However, most of existing studies were based on historical datasets from one environment

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