



CHEMISTRY & BIOCHEMISTRY

SEMINAR PROGRAM

DEPARTMENT OF CHEMISTRY & BIOCHEMISTRY
UNIVERSITY OF OKLAHOMA

NORMAN, OK 73019-3051 ★ (405) 325-4811 ★ FAX: (405) 325-6111

We Are Pleased to Announce A Seminar
Presented By

Giulia Palermo
University of California, Riverside

Monday, May 1, 2023
4:00 pm
SLSRC 3410/3430

*Dynamics and mechanisms of CRISPR-Cas9 through the lens
of computational methods*

The clustered regularly interspaced short palindromic repeat (CRISPR) genome-editing revolution established the beginning of a new era in life sciences. I will report the role of state-of-the-art computations in the CRISPR-Cas9 revolution, from the early refinement of cryo-EM data to enhanced simulations of large-scale conformational transitions. Molecular simulations reported a mechanism for RNA binding and the formation of a catalytically competent Cas9 enzyme, in agreement with subsequent structural studies. Inspired by single-molecule experiments, molecular dynamics offered a rationale for the onset of off-target effects, while graph theory unveiled the allosteric regulation. Finally, the use of a mixed quantum-classical approach established the catalytic mechanism of DNA cleavage. Overall, molecular simulations have been instrumental in understanding the dynamics and mechanism of CRISPR-Cas9, contributing to understanding function, catalysis, allostery, and specificity.

Refreshments will be served