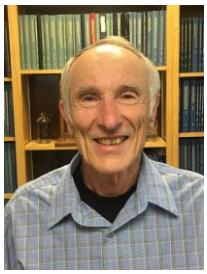

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Quantum Chemistry
Protein Electric Fields
Enzyme Mechanisms
Molecular Dynamics
Protein Fluorescence
Tryptophan, GFPs, RFPs

REPRESENTATIVE PUBLICATIONS

Jianhua Xu, Binbin Chen, Patrik Callis, Pedro L. Muiño, Henriëtte Rozeboom, Jaap Broos, Dmitri Toptygin, Ludwig Brand, and Jay R. Knutson, Picosecond Fluorescence Dynamics of Tryptophan and 5-Fluorotryptophan in Monellin: Slow Water−Protein Relaxation Unmasked, J. Phys. Chem. B (2015) 119, 4230−4239

P.R. Callis, Simulating Electrostatic Effects on Electronic Transitions in Proteins. Molecular Simulation, (2015) 41, 190–204

P.R. Callis, Binding Phenomena and Fluorescence Quenching. I: Descriptive Quantum Principles of Fluorescence Quenching using a Supermolecule Approach, J. Mol. Struct. 1077 (2014) 14-21

P.R. Callis, Binding Phenomena and Fluorescence Quenching. II: Photophysics of Aromatic Residues and Dependence of Fluorescence Spectra on Protein Conformation, J. Mol. Struct. 1077 (2014) 22–29

P.R. Callis, J.R. Tusell, MD + QM Correlations with Tryptophan Fluorescence Spectral Shifts and Lifetimes, Methods Mol. Biol. (Clifton NJ) 1076 (2014), p. 171-214.

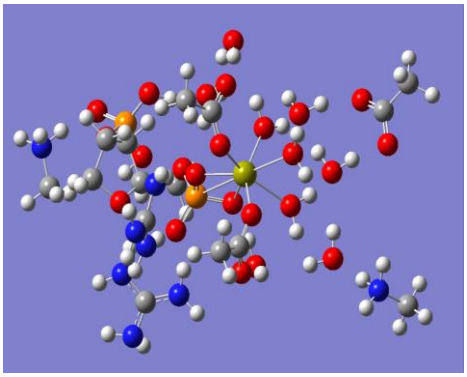
Biesso, J.H. Xu, P.L. Muiño, P.R. Callis, J.R. Knutson, Charge Invariant Protein-Water Relaxation in GB1 via Ultrafast Tryptophan Fluorescence, J. Am. Chem. Soc. 136 (2014), p. 2739-2747.

J.N. Scott, P.R. Callis, Insensitivity of Tryptophan Fluorescence to Local Charge Mutations, J. Phys. Chem. B 117 (2013), p. 9598-9605.

RESEARCH OVERVIEW

Enzymes enormously accelerate the rates of chemical reactions over the rates of the same reactions in water (by 10^8-10^{15} fold), but the precise manner by which enzymes accomplish this in detail is still considered an open question.

We are making a seamless transition from obtaining a detailed understanding of how the intense internal electric fields in proteins profoundly affect the properties of tryptophan fluorescence, towards a better understanding and more detailed view of how enzymes attain their astronomical acceleration of biochemical reactions.



We are currently performing classical and quantum molecular dynamics computations on the active sites of many enzymes, with the goal of observing unbiased enzymatic reaction events.