ACS Local Section
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Computers in Chemistry

Predicting optical properties of molecules in complex environments

Speaker: **Dr. Tim Zuehlsdorff**
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Date: **Friday, May 5, 2023**
Register here (or scan QR code)

Time: 11:00 AM EST
via Zoom

Abstract
Modeling optical properties of complex systems, like solvated dyes, nanostructured materials or pigment-protein complexes is highly challenging, as both coupling of the electronic excited states to nuclear vibrations and explicit interactions with the environment have to be accounted for. In this talk, I will introduce some of the computational methods developed in our research group to address this problem. I will describe the cumulant method, a very successful, albeit computationally expensive approach to calculating optical spectra, that relies on performing molecular dynamics simulations of a molecule embedded in its complex environment. I will then showcase some recent applications of the methodology in our group, including the modeling of solvent-induced changes to the absorption lineshape in the Crystal Violet dye, and understanding the role of pigment-protein interactions in influencing the optical properties of the photoactive yellow protein (PYP). Finally, I will discuss how to model optical spectra with significant contributions from non-Condon effects, such as Herzberg-Teller coupling and conical intersections between multiple excited states, using the example of Methylene blue in solution.

Biography
Tim Zuehlsdorff is an Assistant Professor in Physical Chemistry at Oregon State University. He received his PhD in Theoretical Physics at Imperial College London in 2015. He completed his postdoctoral training at the Cavendish Laboratory at the University of Cambridge (2014-2016) and the University of California in Merced, before joining Oregon State as a Faculty Member in 2020. Tim's research focuses on developing the theoretical approaches and computational methods necessary to understand how complex systems like pigment-protein complexes and nanostructured materials interact with light. He is a contributor to the electronic structure software package ONETEP (www.onetep.org).

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