

# MINI-SCHOOL

# NITheCS

National Institute for  
Theoretical and Computational Sciences

## Modelling optical spectra

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(University of Pretoria)

Attend online: Wed 7, 14, 21 & 28 August 2024 @ 14h00-15h00 SAST

### ABSTRACT

Optical spectroscopy is a ubiquitous tool in many physical sciences, including chemistry, biology, and material science. A thorough understanding of the rich theory underlying spectroscopy is required to interpret and model spectra and develop new spectroscopic methods. In this mini-school, we first briefly revise the quantum-mechanical concepts underlying the description of spectroscopic results, including time-dependent perturbation theory, Fermi's golden rule, spectral line-broadening, and the formation of transition dipole moments. We then discuss the theory underlying linear spectroscopy and derive expressions for the calculation of absorption- and fluorescence-type isotropic, linear dichroism, and circular dichroism spectra. We discuss an exact numerical method and several approximate methods for calculating linear spectra. Finally, we describe the theory underlying nonlinear spectroscopy, and discuss how such nonlinear techniques enable us to follow the quantum dynamics of systems on the femtosecond timescale.

### BIOGRAPHIES



**Prof Tjaart Krüger** is an Associate Professor in Physics at the University of Pretoria (UP). He completed his PhD and a short postdoctoral fellowship at the Vrije Universiteit in Amsterdam where he applied single-molecule spectroscopy to the light-harvesting complexes of plants to understand their exciton dynamics and photoprotective functions. Since establishing a research group at UP, he has extended his research scope to numerous other photosynthetic complexes as well as semiconductors and organic systems, developed experimental laser spectroscopy setups to investigate the molecular details of energy transfer and regulation in these systems, and explored a few theoretical and computational approaches to investigate photosynthetic light-harvesting complexes and organic polymers. He has published over 60 journal articles and supervised over 20 postgraduate students to completion. He is a former executive committee member of the South African Young Academy of Science, a senior editor of the *Journal of Physical Chemistry Letters*, chair of the South African Biophysics Initiative, and a council member of the International Union for Pure and Applied Biophysics.



**Dr Towan Nöthling** received his PhD from the University of Pretoria (UP) in 2023 with a thesis titled *Modelling of Plant Light-harvesting Spectra* under the joint supervision of Prof Tjaart Krüger (UP) and Prof Tomáš Mančal from Charles University in Prague. He is currently a postdoctoral fellow in the same biophysics research group led by Prof Krüger. His research focuses on the use of spectroscopy to describe the ultrafast (sub-picosecond) energy-transfer processes taking place in plants during photosynthesis.

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