2023 Winter Research Project Description

Project title:	**Develop a Matlab app/toolbox to automate optimisation of fitted two-dimensional Electron Paramagnetic Resonance**
Project duration, hours of engagement & delivery mode	Duration of the project, 4 weeks during Summer Vacation. Hours of engagement must be between 20-36hrs per week
Description:	HYSCORE is a two-dimensional EPR technique used to measure electron-nuclear couplings to determine molecular structure around a paramagnetic centre. The couplings are extracted by simulating the HYSCORE spectrum by adjusting the parameters of a spin Hamiltonian model. This project will develop a toolbox or app to automate the optimization of the parameters. Software will be developed in MatLab and various optimisation algorithms can be investigated from non-linear least squares to AI.
Expected outcomes and deliverables:	*Understanding of nuclear magnetic resonance techniques* *Programming skills in Matlab* *Data analysis skill – particularly fitting simulated data to experiment data*
Suitable for:	The project would suit a second or third year student interested in computer programming and applying the techniques to systems in biology and materials science.
Primary Supervisor:	Associate Professor Jeffrey Harmer
Further info:	E jeffrey.harmer@cai.uq.edu.au W http://www.cai.uq.edu.au/harmer