Perturbed angular correlation (PAC) spectroscopy measures the hyperfine interaction experienced by radioactive nuclei that serve as probes in molecular or solid-state systems under investigation. One application of PAC is to measure the electric field gradient (EFG) experienced by probe nuclei in molecules. Within the context of the extended diffusion model, orientations of molecules – and of measured EFGs – change due to (1) inertial rotation and (2) stochastic reorientation of rotation axes caused by molecular collisions. When such changes are on the same timescale as the PAC measurement, the PAC signal exhibits damping. The degree of damping can be used to determine the rate of reorientation or rotational correlation time with use of an appropriate model to relate rotational diffusion parameters to calculation of PAC spectra.

I will use this talk as an opportunity to introduce the PAC method and rotational diffusion. I will describe recent extension of Winkler’s stochastic model for calculating PAC spectra and show its application to determine variation in rotational correlation time of the de novo designed protein TRIL12AL16C in solutions with varying viscosity. I also will present recent work to calculate PAC spectra in the limit where molecular collision rates are much lower than inertial rotation velocity so that measured hyperfine interactions have a harmonic, rather than stochastic, time dependence.

Host: Dr. Gary Collins

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