Facilities

Laboratory:

Kirk Group.

Our research laboratories are located in newly renovated state-of-the-art laboratory space in the Riebsomer wing of the Chemistry Department. There are four research laboratories consisting of: (1) an 1600 sq. ft. preparatory lab which includes segregated desk space for 12 research assistants/associates and associated computers, 3 gloveboxes, 8 hoods, and solvent stills (2) a 2000 sq. ft. shared spectroscopic facility that houses our Raman laboratory, (3) a 1000 sq. ft. laboratory that houses our two UV-Vis-NIR spectrometers and cryostats; an Edinburgh Instruments FLS980 research grade modular fluorimeter; an LP920 laser flash photolysis system (4) a 1600 sq. ft. magnetic spectroscopy laboratory that is dedicated to variable-temperature, variable-field (VTVH) MCD and VT multifrequency EPR spectroscopies. Our Raman system employs PI Acton SpectraPro SP-2556 500mm focal length Imaging Spectrograph with a triple grating turret and PI/Acton Spec-10:100B back-illuminated 1340 x 100 pixel Digital CCD Spectroscopy System with a cryogenically cooled camera head. Coherent Innova Ar+ and Kr+ion lasers, a Coherent Verdi 10W diode pump laser, an MSquared SolsTiS CW titanium:sapphire laser and associated ECD-X frequency doubler provide Raman excitation sources. We also possess a Verdi 10W diode pumped Mira titanium:sapphire laser. This excitation sources allow for essentially continuous wavelength operation in the near-IR and visible regions of the spectrum. Our ability to excite into the red-NIR is of great benefit in the assignment of low energy ligand field and charge transfer excited states, and to avoid fluorescence problems. Our MCD facility consists of Jasco-J700 (UV-vis) and J200 (vis-NIR) spectropolarimeters and a new Oxford Instruments SM4000 8 Tesla magneto-optical cryostat. The MCD spectrometer is built around two Jasco spectropolarimeters that allow us to probe excited states in the 200nm-2.5μ region. The optical configuration is such that the two spectropolarimeters are mounted on a rail assembly, allowing data to be collected in the full 200nm-2.5μ region on the same sample. Our 7 Tesla variable-temperature (1.8-300K), variable-field magneto-optical cryostat is equipped with two sample rod mounted temperature sensors above and below the sample in order to monitor the evolution of any thermal gradients during data collection. All of the support hardware for this instrument is custom designed. We have two Hitachi UV-Vis-NIR scanning spectrometers (U-3501 and U-4100L) and Janis optical cryostats that can be used on CW Raman systems, PL instruments, and for low-temperature (2-330K and 77-300K) optical spectroscopy. All of our laboratory systems are computer interfaced for easy data collection/manipulation.

Office:

Martin L. Kirk possesses an ~400 sq.ft. office on the second floor of the Chemistry Building. This space allows for student meetings and video conferencing.

Major Equipment:

The Kirk Laboratories possess the following major equipment: 1) Raman system consisting of a Spex 1877EP triple monochrometer, Acton Spectrograph, and associated CCD detectors, Coherent Innova Ar^+ and Kr^+ion lasers and a titanium:sapphire-dye laser, 2) MCD spectrometer consisting of Jasco-J600 and J200 spectropolarimeters and an Oxford Instruments SM4000 7 Tesla magneto-optical cryostat, 3) Hitachi UV-Vis-NIR scanning spectrometers, 4) Janis and Oxford Instruments optical cryostats which can be used on CW or pulsed Raman systems and for low-temperature optical spectroscopy, 5) workstations for performing bonding calculations, 6) Two Oxford Instruments 7 Tesla magneto-optical cryostats, 7) Verdi G10 OPSLaser-Diode System (w/ Water Riser and Chiller), Coherent Mira 900-F high-power Titanium:Sapphire ultrafast femtosecond laser, High Power SHG for Mira Femto, 8) Andor Shamrock .3m monochrometer

with an Andor Newton CCD detector and ancillary equipment, 9) Bruker X- and Q-band EPR spectrometers, 10) Edinburgh Instruments photoluminescence spectrometer with time-resolved luminescence capabilities.

Computational Facilities
The Kirk Group maintains several workstations for performing density functional (DFT) calculations using Gaussian, ADF, and ORCA software packages. UNM's Center for Advanced Research Computing (CARC) is the hub of computational research at UNM and one of the largest computing centers in the State of New Mexico. It is an interdisciplinary facility that uses computational resources to create new research insights. The CARC goal is to lead and grow the computational research community at UNM. CARC provides not just the computing resources but also the expertise and support to help the university's researchers. We primarily use "Taos" (Dell R630 Xeon E5-2698 V4 2.20GHz; 23 Nodes; 628 Total cores), "Nano" (Dell PowerEdge 1950; Intel Xeon 5140, 2.33 GHz; 140 Total cores, 1.288 TFLOPS) and "Gibbs" (Dell PowerEdge R620; Intel Xeon E5-2670, 2.6 GHz; 384 Total cores, 3.996 TFLOPS) for these calculations. We make extensive use of these computer facilities to perform detailed bonding calculations (density functional theory (DFT), time-dependent DFT, multireference CI, etc.) using Gaussian, ADF, and ORCA software packages.

Multifrequency EPR Facility
The Kirk group currently maintains the EPR facility in our department. CW capabilities exist on two Bruker EMX EPR spectrometers (with parallel and perpendicular mode cavities) capable of low-temperature EPR (2-300K) measurements at both X- and Q-bands.

Photoluminescence Facility.
The Kirk group shares an Edinburgh Instruments FLS980 research grade modular fluorimeter in the 1000 sq. ft. laboratory that houses our two UV-Vis-NIR spectrometers and associated cryostats. The FLS980 is used to acquire steady-state excitation and emission photoluminescence spectra in the UV-VIS-NIR spectral range for the study of novel electronic and magnetic compounds and materials. The FLS980 was recently upgraded to include time-resolved photoluminescence capabilities (time-correlated single-photon counting; TCSPC).

Magnetic Susceptibility, Magnetization, and Magnetotransport Facility.
This new facility will be supported by UNM's Center for High Technology Materials (CHTM). The PI has recently installed an NSF MRI funded Quantum Design Magnetic Properties Measurement Systems (MPMS) with a liquid helium free Evercool option, which provides state-of-the-art research opportunities in magnetism (Kirk PI). The instrument is used to measure bulk AC and DC susceptibility and magnetization, and magnetotransport properties as a function of applied magnetic field (0-7T) and temperature (1.8 – 300K).

X-ray Absorption Spectroscopy
The Kirk group has a funded proposal to collect XAS and EXAFS data at SLAC-SSRL (Stanford).

Laser Flash Photolysis Facility
The laser flash photolysis instrumentation is located in the Department of Pharmacy on the UNM Medical School Campus and in our electronic spectroscopy laboratory in Riebsomer. The LP920 laser flash photolysis systems (Edinburgh Instruments Ltd) are maintained by Prof. Feng (Pharmacy), and Profs. Kirk and Rack (Chemistry and Chemical Biology). The laser flash photolysis data can be obtained in both spectral and kinetic modes. These instruments can be used to measure fluorescence, rapid kinetics of electron transfer, and transient absorption spectra (ns to seconds timescale).

Mass Spectrometry Facility
The UNM Mass Spectrometry Facility is housed in the Department of Chemistry and Chemical Biology, and provide mass measurements for small molecules, analysis of protein patterns in disease, materials characterization, etc. We use this facility extensively in support of our synthetic endeavors. A recent addition to the facility is an NSF MRI funded GC Q-ToF MS (Kirk co-PI).

Small Molecule X-ray Crystallography Facility
The UNM Chemistry Department shares an X-Ray Laboratory with Sandia National Laboratories at UNM's Advanced Materials Laboratory. The facility possesses a Bruker X8 APEX Single-Crystal X-Ray Diffractometer with high sensitivity CCD detector, which serves the structure determination needs for the department, the University and other institutions.

Center for Integrated Nanotechnologies (CINT)
This facility is located in Albuquerque, just a few miles from UNM, and at Los Alamos. World-class facilities exist for time-resolved optical spectroscopy, Raman and infrared spectroscopy, cryogenic and magnetic fields used in combination with optical spectroscopies. The ultrafast laser spectroscopy facility in Albuquerque possesses fs transient absorption and photoluminescence spectrometers operational at wavelengths from the ultraviolet to the far-infrared. CINT facilities for TRIR are located at the Albuquerque and Los Alamos Gateways.

Other Resources
The Department maintains a large NMR facility that we use for characterization of small molecules. The physical sciences library is adjacent to the Chemistry building.