Christine Beavers, Research Scientist, Beamline 12.2.2 at the Advanced Light Source.

Supervised by Quentin Williams, UC Santa Cruz

June 1st, 2013-Current (3 years, 5 months)

Responsibilities include developing/running the single-crystal diffraction experiment and facilities (70%) and providing on-site support to COMPRES users (20%) and non-COMPRES single-crystal users(10%). I have supported the groups of Williams(UCSC), Ross(VTech), Jackson(CIT), Karunadasa(Stanford), Olmstead(UC Davis), Alivisatos, Long, Yaghi(UC Berkeley), Tolbert(UCLA) & Ciezak-Jenkins(Army). Although some of these groups are not COMPRES, they require my expertise in some facet of collecting single crystal data on 12.2.2. I have also supported the Williams group, and others, when collecting data on beamline 11.3.1, which is the small molecule crystallography beamline.

My single crystal time this year has been split between optimizing data collected on the current system and preparing the new system. Over this last year, I have conferred with George Sheldrick, to understand some systematic issues with 12.2.2 data. With his help, I have determined that using the Diederich method, to understand the collected intensities, allows us to now solve and refine most data sets from the Perkin Elmer on 12.2.2. This improvement has vastly improved the odds of success when doing a single crystal experiment. The Stoe Stadi-Vari 4-circle diffractometer, equipped with an RDI CMOS fast detector, was installed last March, and has been in a commissioning state with an unfocused X-ray beam, which has allowed me to optimize the data collection routines and analysis methods. The diffractometer will be placed upon the rugged stages, purchased on the EOID award, in mid-December, which will allow us to place the diffractometer on a focused beam. A Labview routine is being developed, to my specifications, to allow the images from the new system to be analyzed in almost any commercial single crystal software package. Over this upcoming ALS shutdown, which runs from late Dec to mid-March, the single crystal diffractometer endstation will be finalized, and it should become open to general users Spring 2017.

I am involved with numerous projects concerned with single crystal HP, with groups around the country and the world. The Williams group at UCSC is continuing to work with me and other beamline staff to implement HPHT single crystal, and this development will accelerate once the diffractometer is on a focused beam. The Karunadasa group at Stanford has recently published a major HP single crystal paper on lead halide perovskites, with others forthcoming. Professor Simon Parsons, of the University of Edinburgh, has entered into partnership with the ALS, which has allowed him to send a student to be a resident doctoral fellow. The Parsons group is well known as one of the premier molecular high pressure research group; this student has been working with me to utilize 12.2.2 and 11.3.1 for single crystal high pressure experiments. I have also assisted numerous other groups in writing beamtime proposals,

I have been very active in outreach this year. I consider my outreach work to fall into two categories: technical outreach and broader science outreach. Technical outreach is what I consider identifying our potential user base, and reaching out. Attending conferences, such as the American Crystallographic Association meeting and the European Crystallographic meeting, count to me as technical outreach. I attended both of these meetings to advertise our technical capablities and expand our potential user base. At both conferences, I met many scientists interested in high pressure single crystal, and some of these contacts will be submitting proposals for 2017-2. Broader science outreach includes education on our technical capabilities, but in a longer term sense- my lecturing at the National School on Neutron & X-ray scattering is more educational, less advertising. My lecture this year was again well received, and numerous students were intrigued by the concept of HP diffraction. I was also invited to lecture at next year’s ACA Crystallography summer school, where many COMPRES faculty have sent their students. I also represented crystallography, and the ACA, at the quadrennial meeting of the Society of Physics Students, Physcon. This large event was a great opportunity to introduce students to the power of crystallography, and many were surprised that they had never encountered this technique in their studies.

Publications (2015-2016)

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