Application Title: New High-Energy X-ray Diffractometer

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Key Participating Units: College of Arts and Science, College of Engineering, School of Public Health

Anticipated Request Amount ($): $749,800

Executive summary of this application to utilize Research Development Funds:

We are requesting funds to support the purchase of a new dual Ag/Mo X-ray diffractometer. Crystallography based structure elucidation is a key component to developing atomistic understanding of matter that underpins wide ranging scientific efforts in chemistry, materials science, geoscience and the life sciences. The fundamental importance of knowing composition and connectivity of a system is reflected in the intimate connection between general scientific advancements and X-ray science breakthroughs that is perhaps best epitomized by synchrotron facilities. Synchrotron science is well-represented in some of the leading breakthroughs from Texas A&M (structure elucidation of metal-organic frameworks for catalysis, visualization of reactive intermediates in small molecule activation, temperature dependent response of molecular gyroscopes). However, "beamtime" at these facilities is an inherently limited resource that requires proposals, travel and scheduled experiments that are both vulnerable to external sources of uncertainty such as upgrades and access restrictions and not always compatible with the rapidly evolving and changing nature of research.

Crucially, recent advancements in detector technology efficiency and X-ray source brightness enable in-house crystallography experimentation that was previously only accessible at such facilities. Specifically, we are proposing to acquire a new diffractometer using a dual Ag/Mo source that will allow for the collection of synchrotron-like data. In addition to providing that capability, it will also upgrade obsolete instrumentation and enable the collection of diffraction data at significantly shorter wavelengths than previously supported. This instrument includes a new detector with immensely improved sensitivity that will broadly support enhanced structure elucidation technology across facility users and ensure resiliency in our services that currently rely heavily on completely subscribed but aging infrastructure. Furthermore, this combination of a bright, high energy source and a sensitive detector allows experiments in specialized set-ups for probing atomic behavior under extreme conditions, as well as diffuse scattering experiments that are otherwise not supported at Texas A&M at this time. Together, these capabilities introduce the tantalizing possibility of turning experiments previously only possible at dedicated synchrotron beamlines into routine structure elucidation studies, accelerating the feedback loop between experimentation and results, and propelling science across the aforementioned disciplines.

Historically, Texas A&M has prided itself on the strength of its diffraction facilities, with key proponents such as the late Prof. F. Albert Cotton who recognized early on the importance of maintaining cutting edge capabilities. The instrument described in this proposal is exactly that, representing the forefront of in-house diffraction capabilities while also serving the broad needs of facility users. To the best of our knowledge, there are no equivalent instruments in academic institutions in the state of Texas further exemplifying the power of this acquisition to introduce unique and competitive capabilities