

## SMS 2023 P&T Seminar

Friday Sept 1 | 1pm | Biodesign Auditorium

### Tuning the Ultrafast Energy Flow in Molecular Scale Materials

Clusters and related (sub)-nanoscale systems are promising alternatives to traditional bulk materials as they often exhibit novel properties, stemming from their quantized sizes, that can be developed for energy conversion applications. I will present our recent ultrafast spectroscopy measurements that demonstrate the exquisite tunability of the physical and chemical properties of clusters, through systematic adjustment of their atomic composition, enables new understandings to control energy flow. By tuning the d-electron density of strongly correlated, neutral metal oxides clusters with atomic precision, our ultrafast measurements act as a window to monitor electron correlation and identify the structural features driving carrier localization/separation and polaron formation.<sup>1,2</sup> We developed an innovative technique for quantifying the metallicity of molecular sized materials.<sup>3,4</sup> The electronic relaxation properties are strongly dependent on both size and local structure, enabling sub-nanometer clusters to exhibit metallic or semiconducting properties, and even transition between the two in direct relation to the ligand-to-metal charge transfer (LMCT) character of the photoexcitation. I will also present new results on the ultrafast ion-pair formation photodynamics of small atmospheric molecules, which have attracted substantial attention due to their prominent role in acid-base chemistry, ozone depletion and acid rain. Nonadiabatic relaxation following Rydberg state excitation in small molecules operates as a multistep process reaching an intermediate state within ~500 fs and finally predissociation to the ion-pair  $[C_4H_9^+ - Br^-]$  state within  $10.8 \pm 0.5$  ps.<sup>5</sup> We find that excited state proton transfer and ion pair formation is an important protection mechanism that stabilizes small formic acid clusters  $(FA)_n$  against ultraviolet photodissociation on the fs timescale. However, proton transfer becomes exponentially less favorable with decreasing size, explaining why it has never been seen in  $FA_2$ .

### Scott Sayres, PhD

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Scott G Sayres is an Assistant Professor in the School of Molecular Sciences and Biodesign Center for Applied Structural Discovery at Arizona State University. He obtained a B.S. in Mathematics and Chemistry from Shippensburg University in 2004. He then earned a Ph.D., working with A. W. Castleman Jr. at Penn State, on the strong-field interaction of light and matter and then worked on attosecond transient absorption spectroscopy as a postdoctoral fellow at UC Berkeley with Stephen Leone. His research interests focus on the development of novel nanostructures with atomical precision and stabilizing light-induced states in quantum materials. Controlling such nonequilibrium physics can make a transformative impact on the realization of next generation photocatalysts and quantum technologies.



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Co-organizer of 2025 Symposium on Size Selected Clusters

\*ZOOM option available: <https://asu.zoom.us/j/84890997395>