Self-driving Lab for the Photochemical Synthesis of Metal Nanoparticles with Targeted Size, Shape and Composition

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Many applications of metal nanoparticles (NPs) require precisely controlled optical properties that are governed by the NP shape, morphology and composition. Finding reaction conditions for the synthesis of NPs with targeted characteristics is a time-consuming and resource-intensive trial-and-error process, however closed-loop NP synthesis enables the accelerated exploration of large chemical spaces without human intervention. Here, we introduce the Autonomous Fluidic Identification and Optimization Nanochemistry (AFION) self-driving lab that integrates a microfluidic reactor, in-flow spectroscopic NP characterization, and machine learning for the exploration and optimization of the multidimensional chemical space for the photochemical synthesis of metal NPs. By targeting spectroscopic NP properties, the AFION lab successfully identified reaction conditions for the synthesis of different types of NPs with designated shapes, morphologies, and compositions, including gold tetrapods that have not been previously synthesized via seedless photochemical reaction. Data analysis provided insight into the role of reaction conditions for the synthesis of the targeted NP type and the impact of a specific condition on NP quality. This work shows that the AFION lab is an effective exploration platform for on-demand synthesis of metal NPs.