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Using Operando Characterization, Data Analytics, and Artificial Intelligence to Understand Mechanistic Links between Processing and Structure

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In this presentation, we will describe a vision for a future research paradigm, wherein a tight coupling of in-situ and operando experimental methods, data analytics and automated data analysis are coupled with artificial intelligence to direct how we use electron microscopy (and other forms of materials characterization) to characterize the mechanisms by which processing/structure/property relationships are determined. The presentation will be forward looking and will incorporate research results and ideas culled from a variety of sources and authors: it will not be a typical presentation reviewing research from just the co-authors.

First, we will describe the motivations for working towards this type of research paradigm. These include the desire to speed up the rate of scientific discovery and time to market, as well as a more pedestrian desire to maximize the utilization of expensive instrument time.

Second, we will review examples of autonomous research methods, both through data mining of the literature [1,2], and through the use of real time feedback and artificial intelligence methods to direct experimental outcomes.[3] Specifically, we will discuss how these approaches may be utilized in electron microscopy research in the near future, and the developments needed to bring this to reality.

Third, we will describe how this approach can be used to explicitly and efficiently test operative hypotheses, and to efficiently understand the relevant experimental parameter space. This yields insight as to where detailed experimentation is most valuable. In this portion of the talk, the need for operando methods and correlative experimentation will be emphasized.[4]

Finally, we will discuss this evolving research paradigm as it exists both within and provides challenges to established theories of scientific discovery.[5,6]

[1] Chaomei Chen, J. Data and Inform. Sci., **2**, 2017, pp. 1-40.
[2] http://cluster.cis.drexel.edu/~cchen/citespace/
[3] P. Nikolaev, et al., npj Comp. Mater., **2**, 2016, 16031.
[4] Y. Li, et al., Nature Comm., **6**, 7583 2015.
[5] The Structure of Scientific Revolutions, T.S. Kuhn, Chicago: University of Chicago Press, 1962.
[6] S. Fuchs, Social Forces, **71,** 1993, pp.933-953.

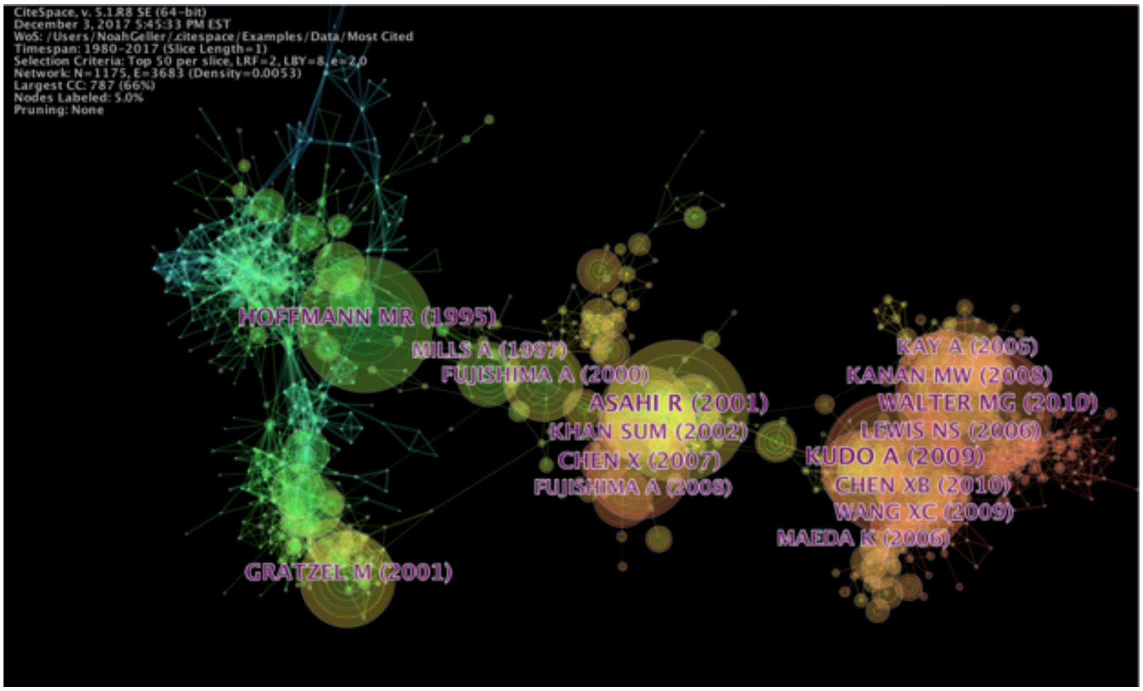

Figure 1: Example output from Citespace analysis [1,2] using the output of a Web of Science search using keywords *photocatalysis*, *photoelectrochemistry*, *solar fuels* and *water splitting*

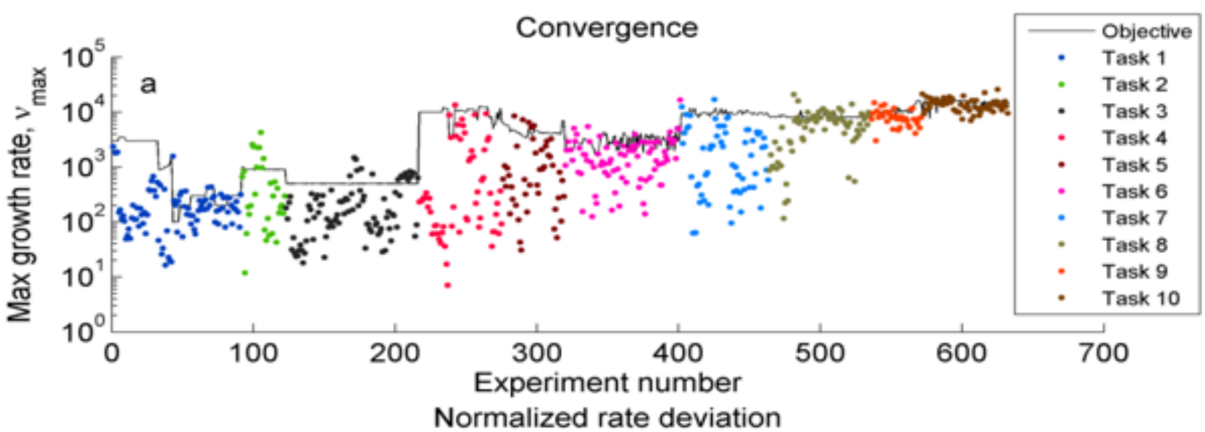

Figure 2: Example of autonomous experimentation guiding the growth of carbon nanotubes towards maximum growth velocity. From [3]

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