ALCF SDL WORKSHOP (2019)

Argonne NATIONAL LABORATORY

UV/VIS ABSORPTION SPECTRA DATABASE AUTO-GENERATED FOR OPTICAL APPLICATIONS VIA THE ARGONNE DATA SCIENCE PROGRAM

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October 2 (2019)
ANL

DATA-DRIVEN MOLECULAR ENGINEERING OF SOLAR POWERED WINDOWS

ALCF Data Science Program (ADSP)

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- Edward J. Beard (PhD Student)

Argonne Leadership Computing Facility, Argonne National Laboratory

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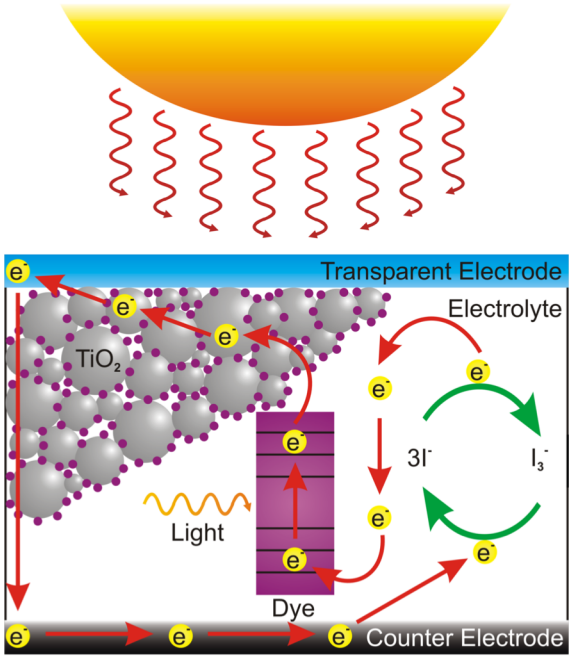
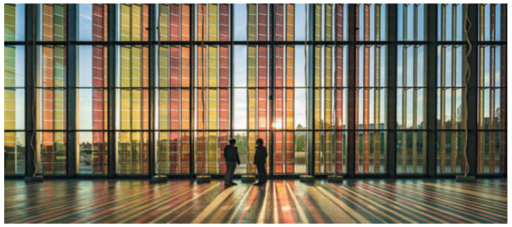
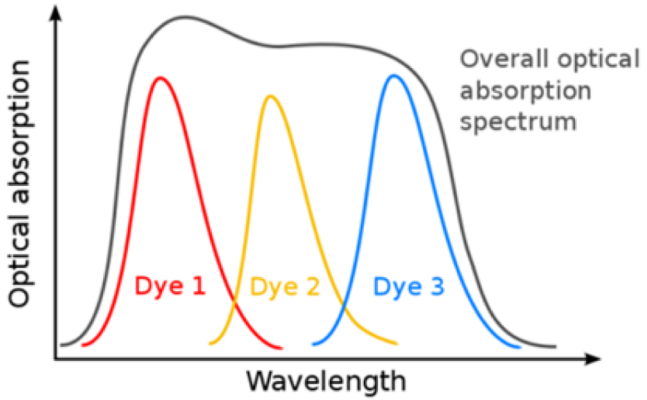
- Venkatram Vishwanath, Manager (ADSP Program)

- **ALCF Theta**

SOLAR-POWERED WINDOWS



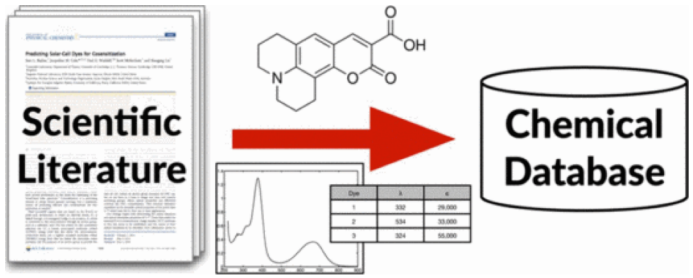




Maximizing light harvesting efficiency

Rules: LUMO > Ec_{TiO2} , HOMO < $E_{electrolyte}$

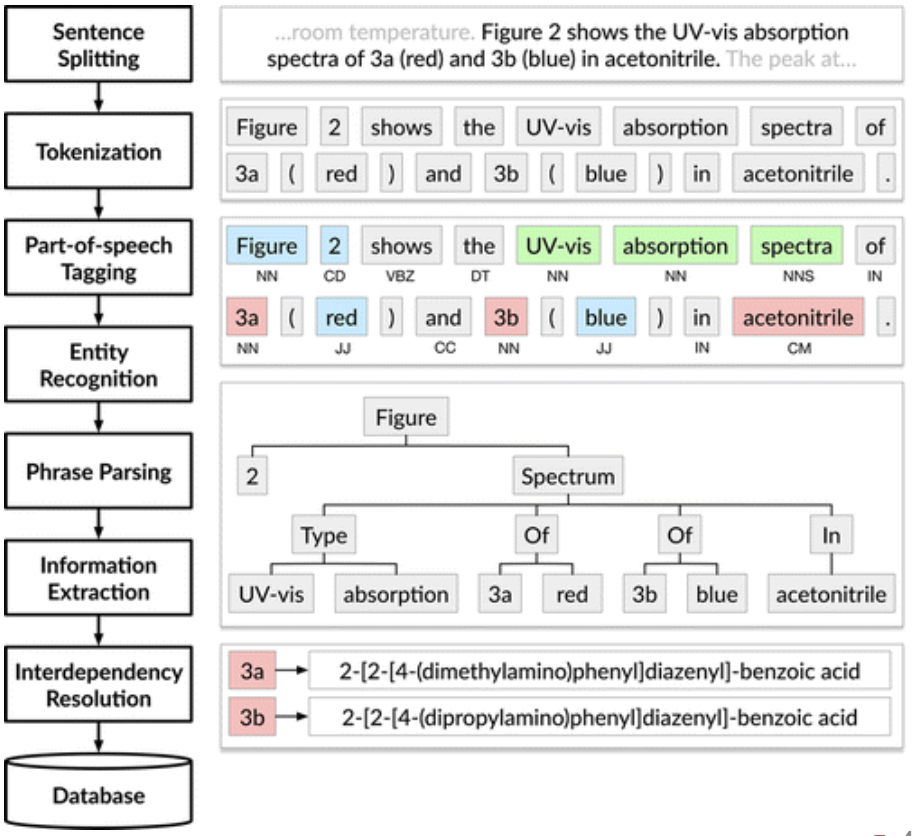
CHEMDATAEXTRACTOR[1]



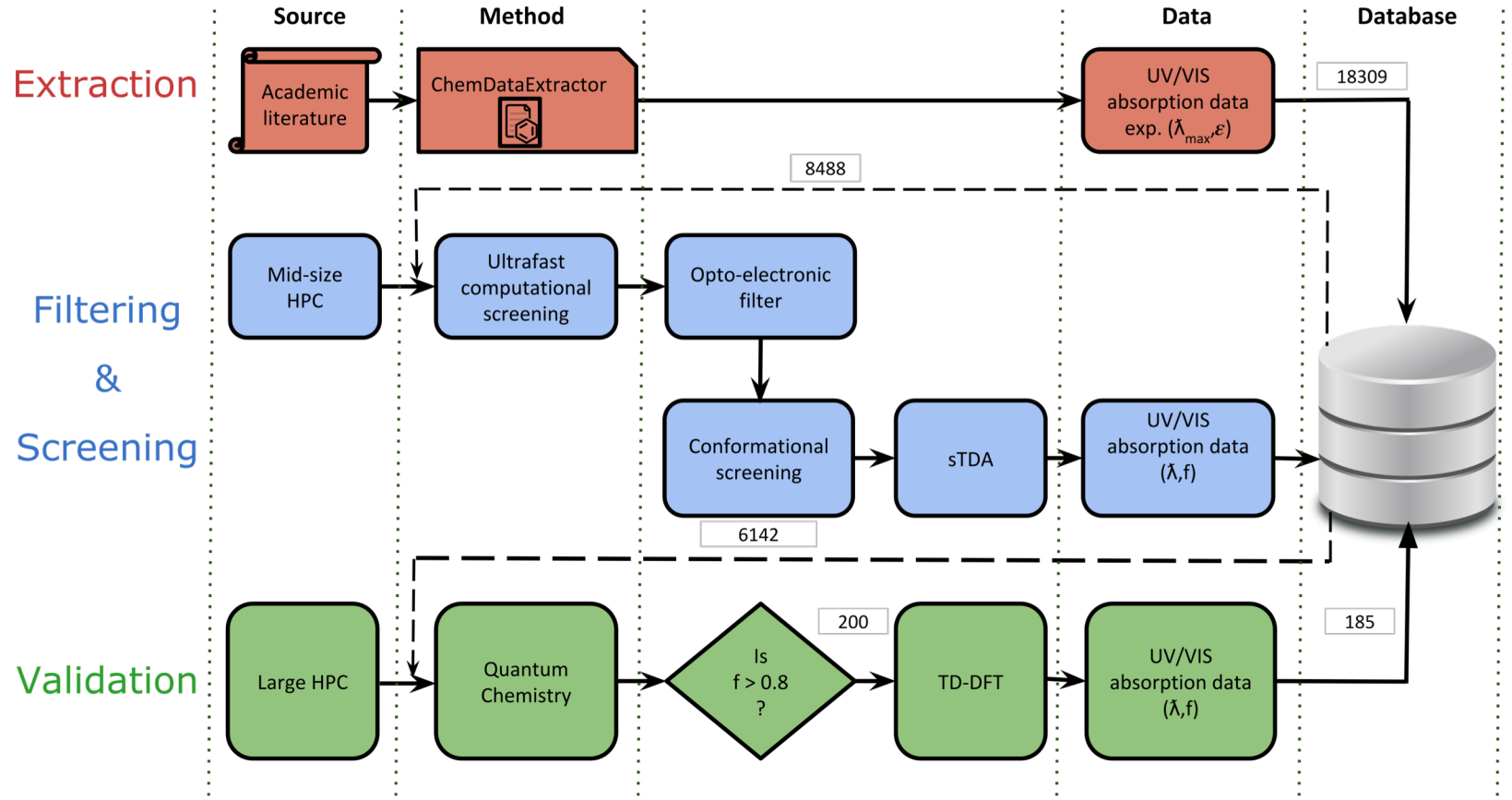
- Natural language processing and data-mining :

- An initial corpus of ~ **400,000** scientific literature.

[1] http://chemdataextractor.org/

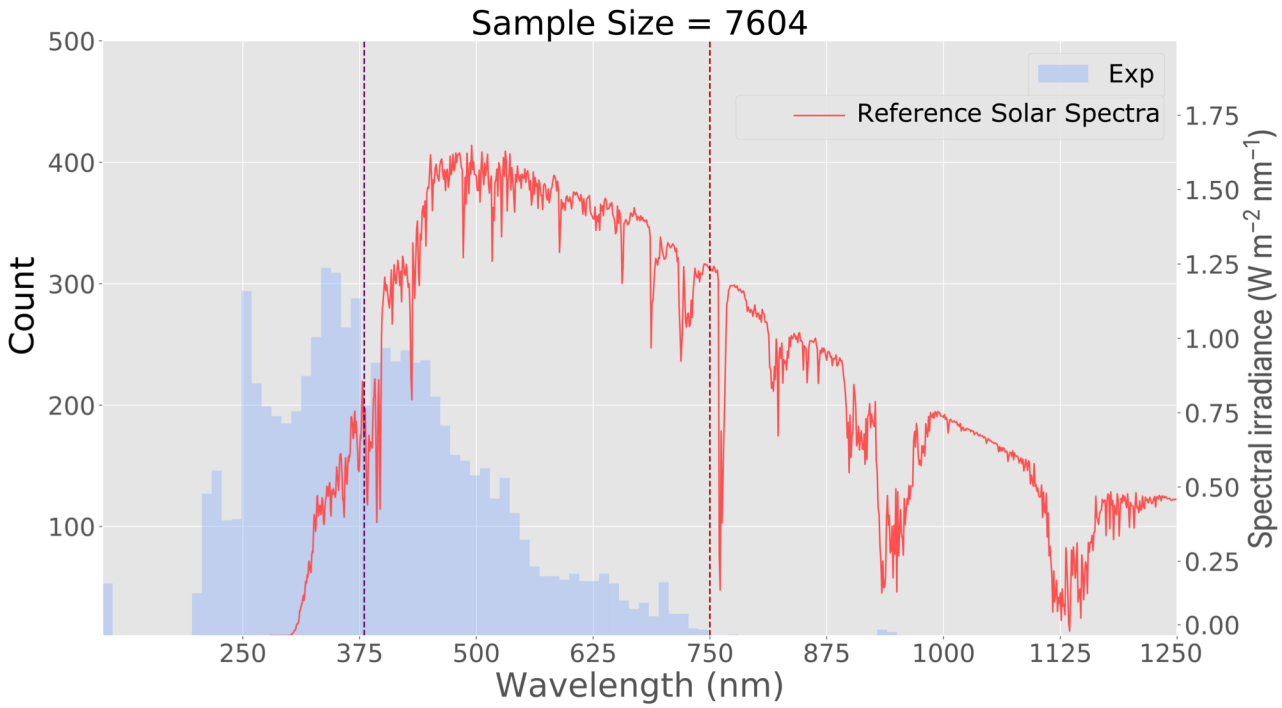


AUTOMATED HPC WORKFLOW FOR FUNCTIONAL MATERIALS

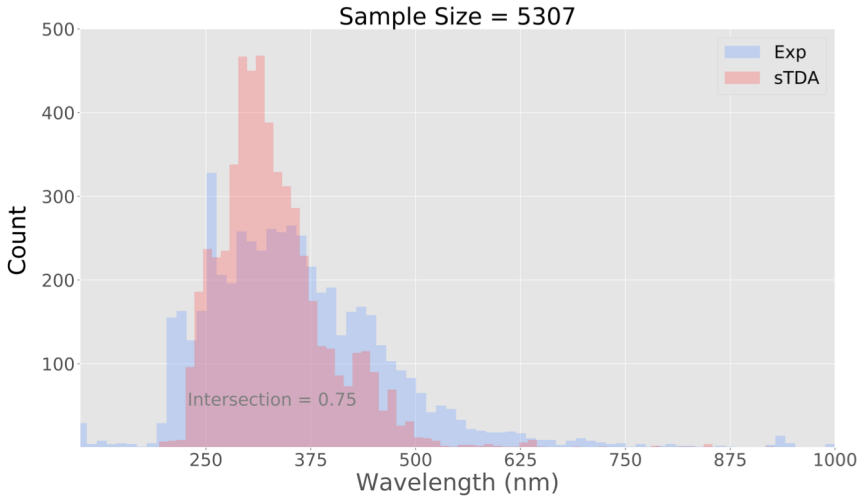


TECHNICAL VALIDATION

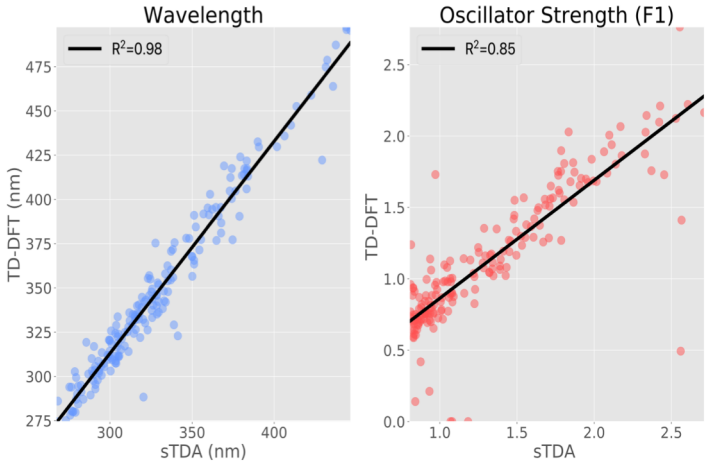
WAVELENGTH DISTRIBUTION



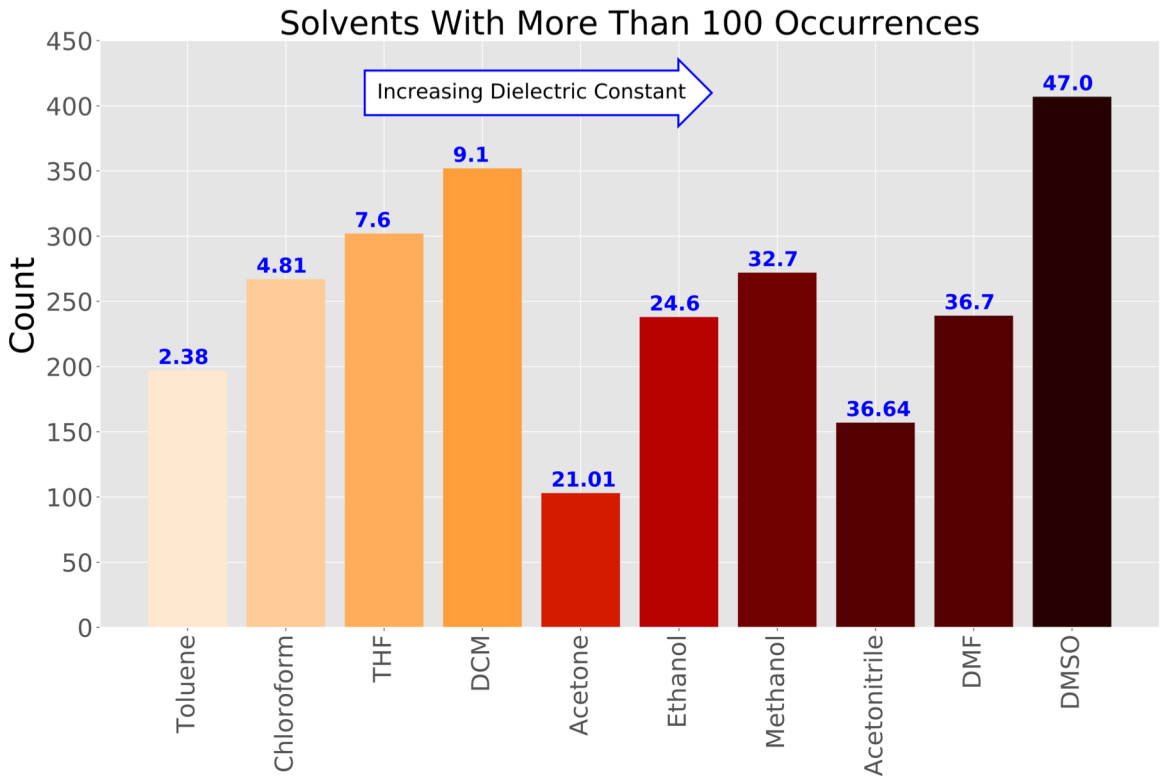
EXPERIMENT VS THEORY



COMPARE THEORY



TOP SOLVENTS REPORTED IN LITERATURE

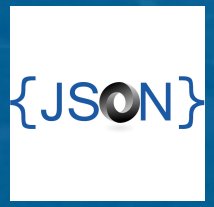


OUTLOOK

- 1000+ compounds with large oscillator strength.
- Identify candidates for DSSC.

Rules: $LUMO > Ec_{TiO2}$, $HOMO < E_{electrolyte}$

E. J. Beard,G. Sivaraman, Á. Vázquez-Mayagoitia, V. Vishwanath, J. M. Cole, ***Comparative dataset of experimental and computational attributes of UV/vis absorption spectra***, Sci. Data. (In Review)



THANK YOU!
QUESTIONS?

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