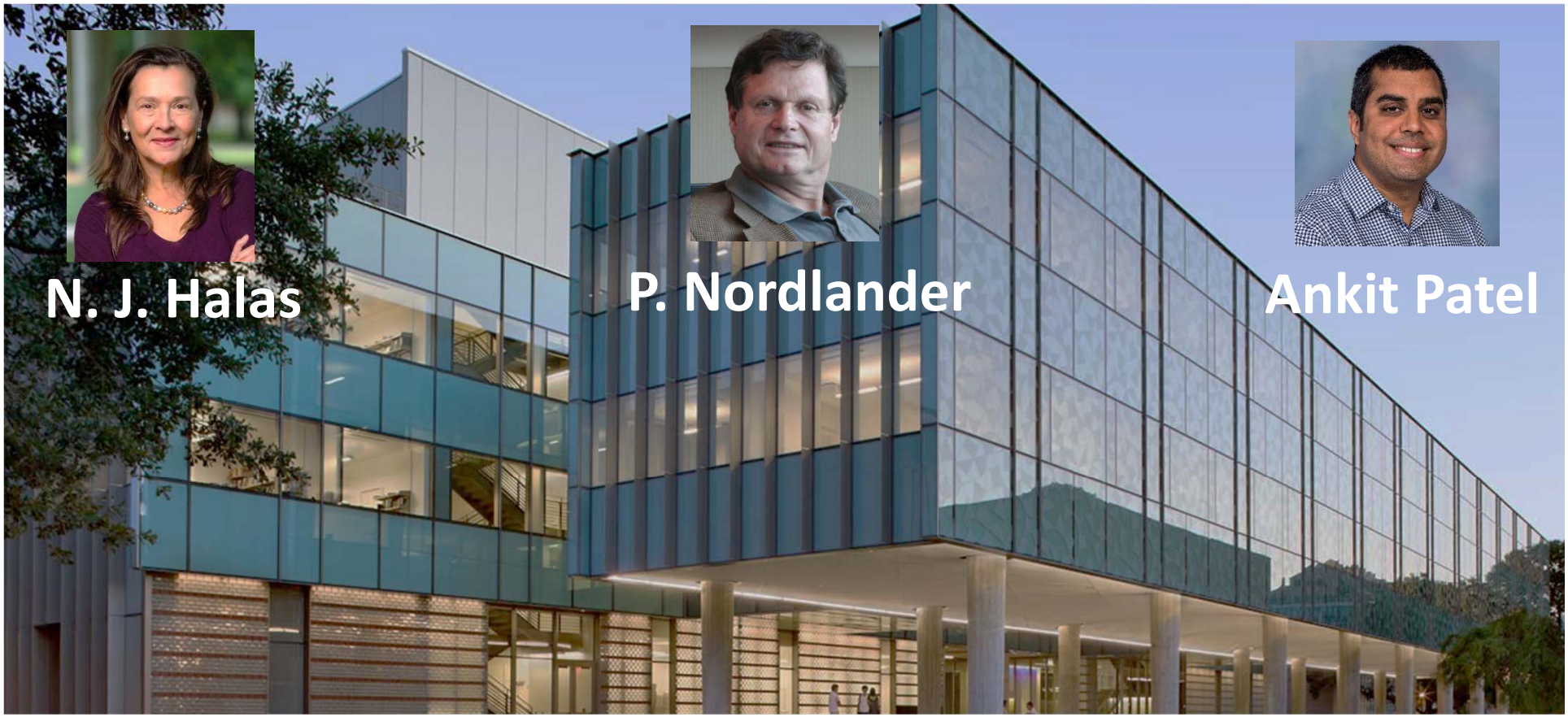
Project 1:

Streamlined identification of PAHs/PACs using ultracompact spectroscopy and machine learning



Hypothesis

Streamlined, fieldable methods for PAH and PAC* detection and identification will revolutionize our assessment of:

- public degree of exposure,
- patient pathology, and
- remediation efficacy,

for this dangerous family of chemicals.

*PACs are original PAHs that are chemically modified: they are more soluble in water and can be taken up more easily into living tissue and cells than PAHs.

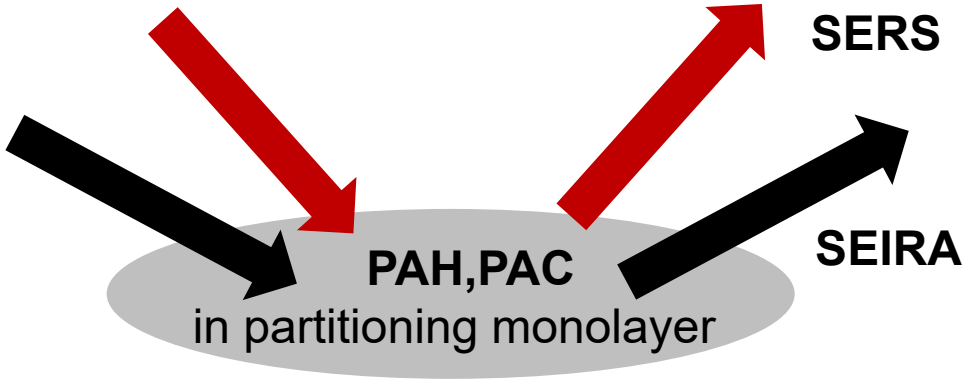
The detection challenge:

- Both **detection** and **identification** are needed to assess PAHs AND their PAC derivatives
- PAH, PACS typically found in complex mixtures
- “Gold standard”: laboratory-based detection methods are costly and time-consuming
- “Gold standard” approaches are LARGE: not translatable to portable or fieldable platforms

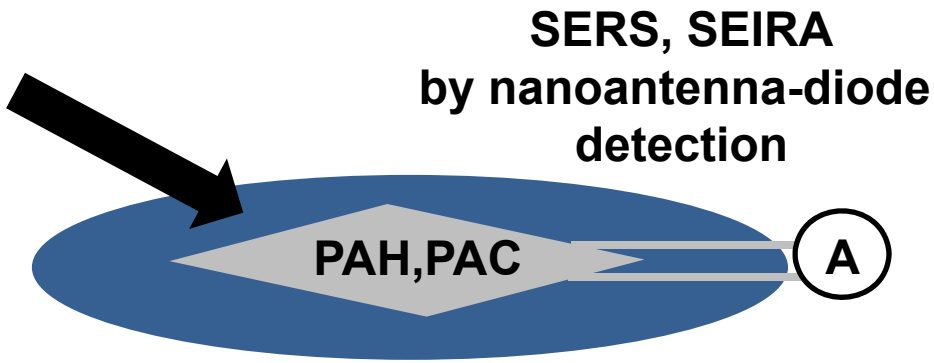
Specific Aims

1: High-sensitivity PAH, PAC detection using Nanoparticle-enhanced spectroscopies

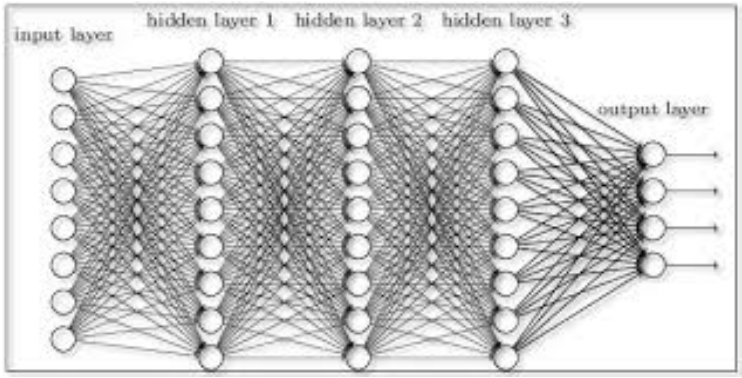
2: Identification of PACs combining Raman and IR enhanced spectroscopies



3: Ultracompact detector/analyzer for PAH/PACs based on electronic detection



4: Identify PAHs, PACs in multicomponent samples using machine learning strategies



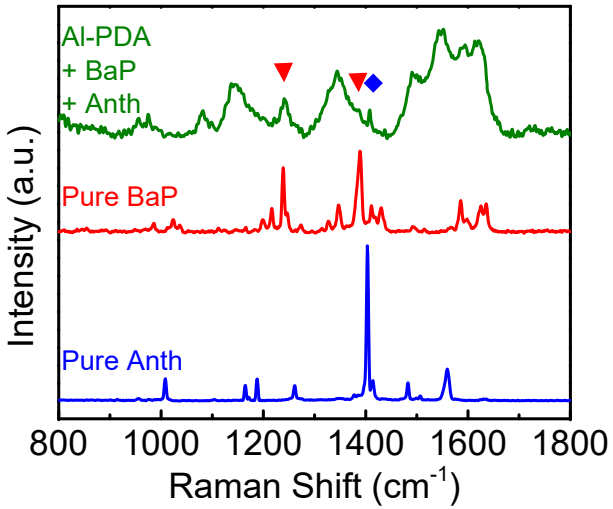
Our approach

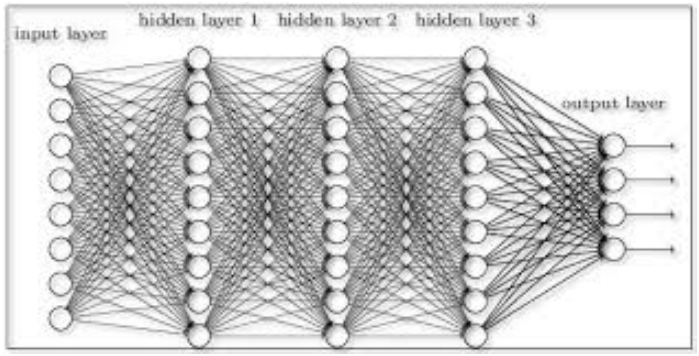
- Compile libraries of PAH/PAC spectra
- Train machine-learning methods like *convolutional neural networks* with measured spectra
- Algorithms will enable identification of PAH and PAC components from multicomponent spectra

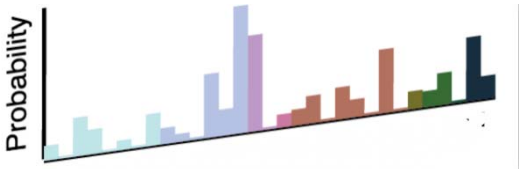
Input: multicomponent Sample spectra

ML method/convnet

Output: Types of PAH, PAC molecules identified







Anticipated Project Outcomes and Impact

A new capability for rapid identification of PAHs and PACs

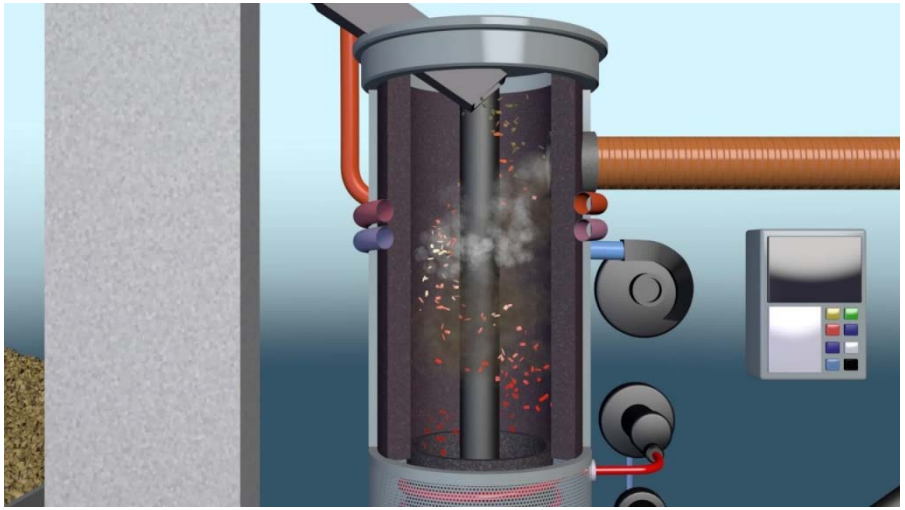
- Compact
- Fieldable
- Rapid compared to current methods
- Capable of PAH/PAC identification in complex mixtures

Project 4:
Pyrolytic Treatment of PAH- Contaminated Soils to Eliminate Toxicity and Enhance Fertility

Pedro J.J. Alvarez and Kyriakos Zygourakis
Rice University

22 May 2020

Pyrolysis



- Thermal decomposition in an inert (anoxic) atmosphere.

- Widely used to make biochar from wood, and to produce ethylene & other chemicals from petroleum or coal (including coke).

Biomass → Tars + Volatiles + **Biochar**

Rice Husk

Pyrolysis of contaminated soil represents a novel application

Hypothesis

Pyrolysis of soils impacted by PAHs quickly desorbs or converts pollutants into char-like material, meeting cleanup standards, eliminating toxicity and enhancing soil fertility.

Excavate

Pyrolyze

Revegetate

Modified TD Unit

Objectives

1. Test the hypothesis that pyrolysis will efficiently and broadly remove PAHs and other hydrophobic priority pollutants, and eliminate their toxicity.

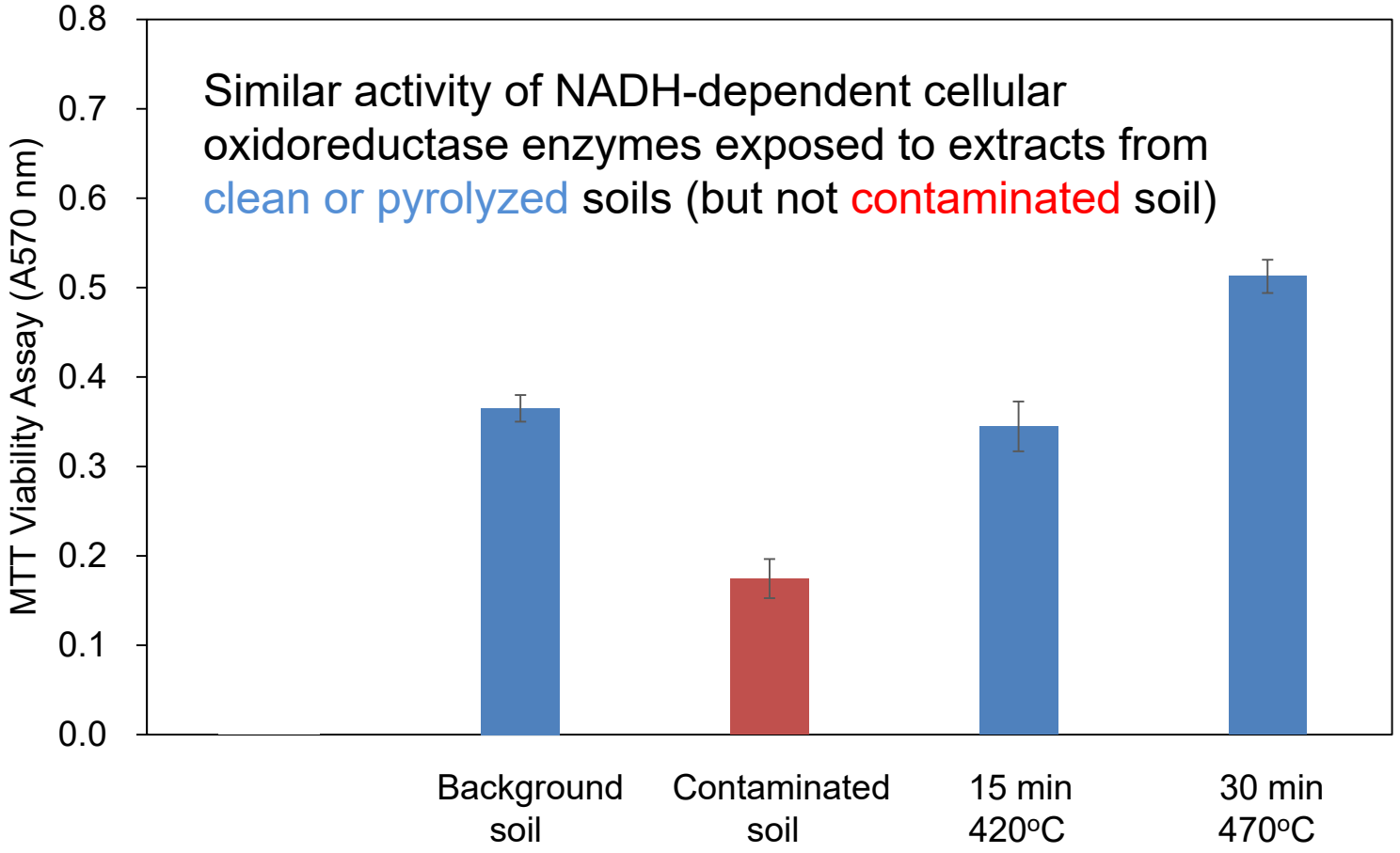
2. Characterize the reaction mechanisms (including catalytic role of clays) and end products to guide safe, reliable and cost-efficient application.

3. Identify/model the operating conditions that maximize the benefits of soil pyrolysis (reliable and efficient remediation and improved soil fertility) while minimizing associated costs.

Pyrolyzed (420°C)
TPH: N.D.

Untreated
TPH: 15,000 mg/kg

Effective Detoxification (Human Lung Cells)



Song W., J.E. Vidonish, P. Yu, C. Chu, B. Moorthy, B. Gao, K. Zygourakis and P. Alvarez (2019). Environ. Sci. Technol. 53:2045-2053.

Anticipated Conclusion (we hope to prove)

Different treatment objectives (regulatory compliance, detoxification, & soil fertility restoration) need not be mutually exclusive, and could be simultaneously achieved with appropriate pyrolytic treatment intensity (controlled through pyrolysis temperature and residence time).