DuraMAT
Durable Module Materials Consortium

Materials Discovery and Forensics Capability 3: Developing an applied materials discovery workflow

Capability Lead: Mike Toney - SLAC National Accelerator Laboratory

Initial Team Members:

Simulation: Steve Follies (Sandia)

Synthesis: Bryan Kaehr (Sandia), Andriy Zakutayev (NREL),

Characterization: Margaret Gordon (Sandia), Laura Schelhas and Mike Toney (SLAC)

"The overarching goal of DuraMat is to ***discover, develop, de-risk****, and enable the rapid commercialization of* ***new materials*** *and designs for photovoltaic (PV) modules with the potential to improve performance and lifetime while achieving a levelized cost of electricity (LCOE) < $0.03/kWh"*

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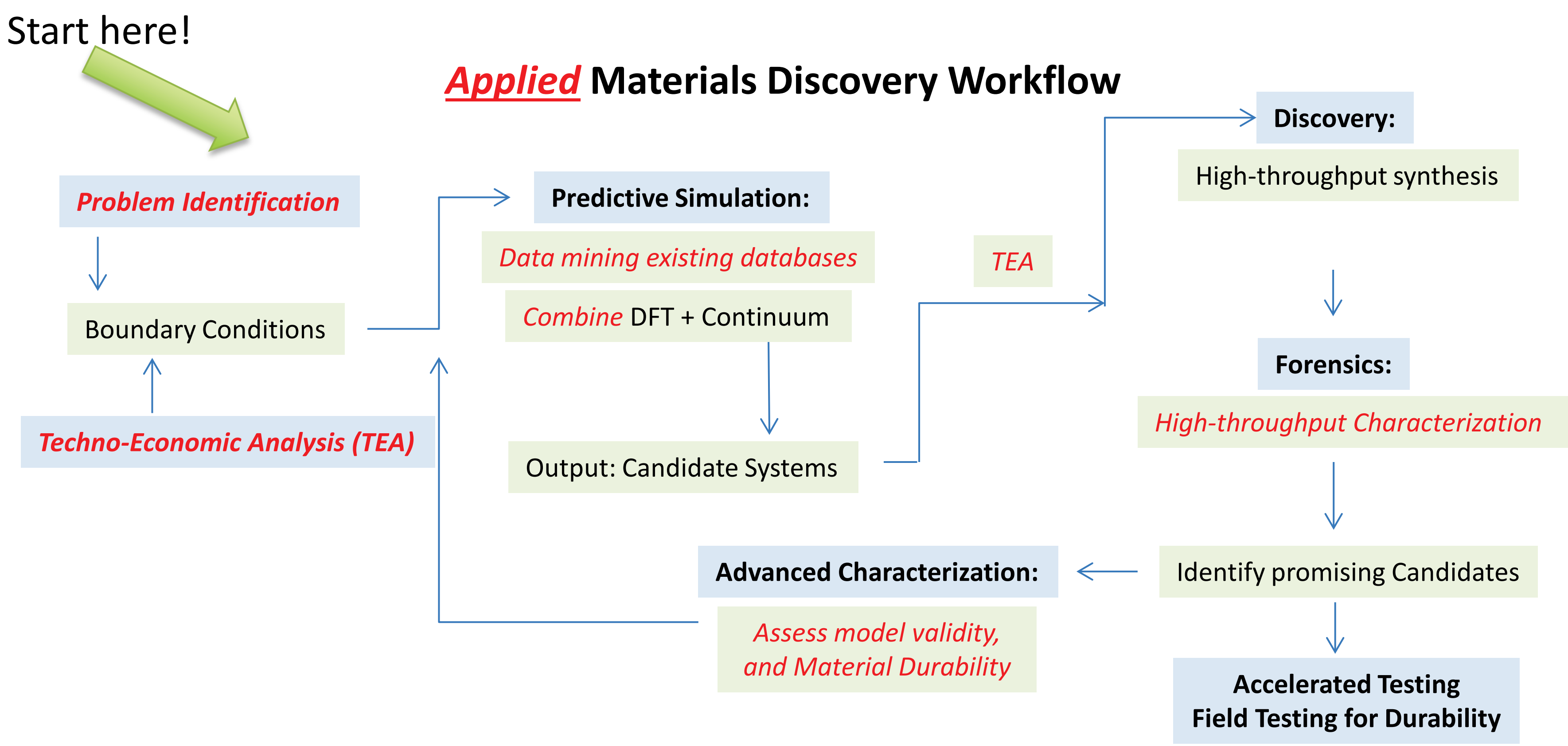
Goals, approach, results: Materials Discovery and Forensics

- Develop a broad set of **pre-competitive** module materials
  - Cost, performance & manufacturability as a key design criterion (materials discovery)
- Approach: Build and demonstrate a tool set with a relevant test case to show applicability
  - High-throughput synthesis & characterization & computation
  - Forensics of failure & degradation
- Result: robust materials discovery and development platform
  - **rapid** & **cost effective**
  - focused on **module materials**

Applied Materials Discovery Workflow



What will this capability development provide? (Highlighted in red)

1. Integrate DuraMat capabilities
   -Facilitate development of feedback loops/communication in capability network
2. Hardware: High-throughput contact angle, Combi-soiling stage design

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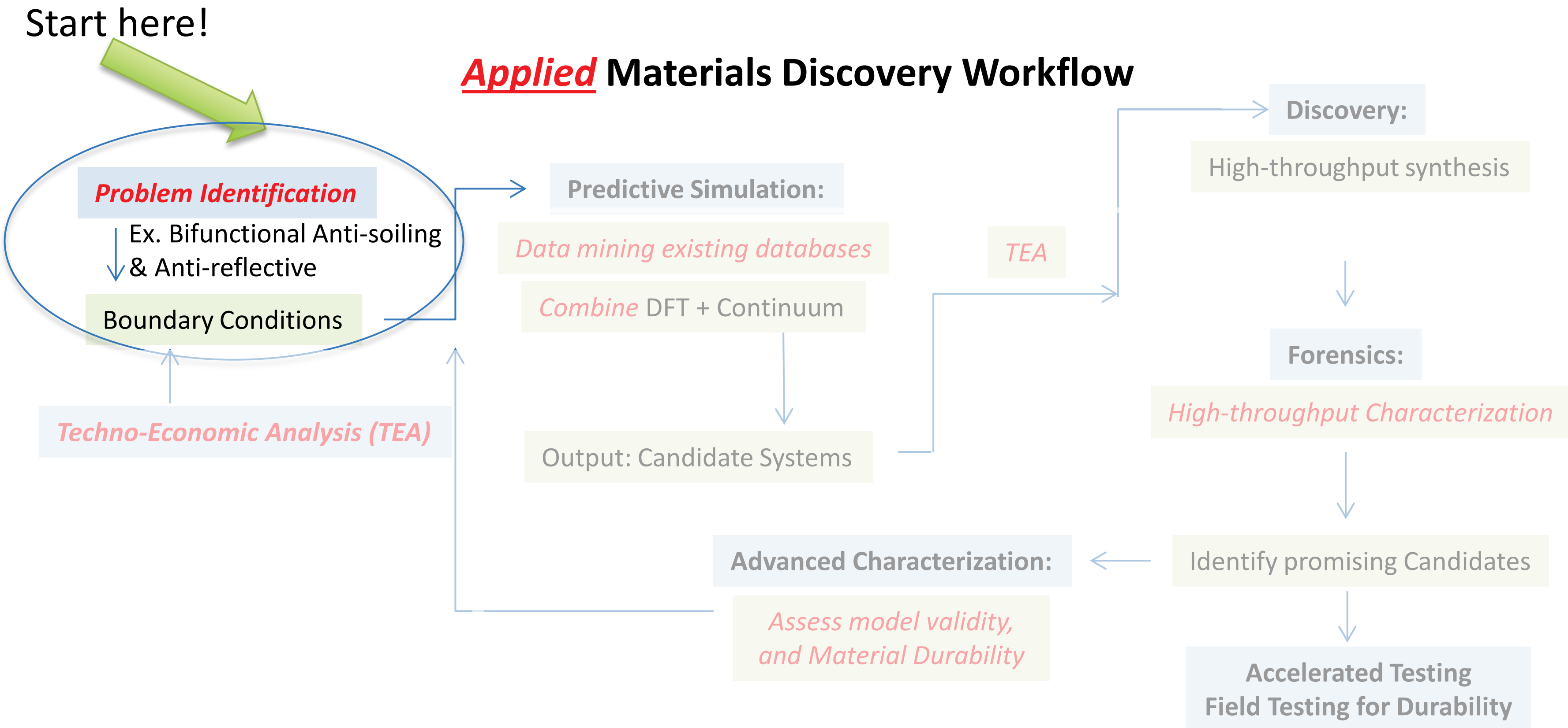

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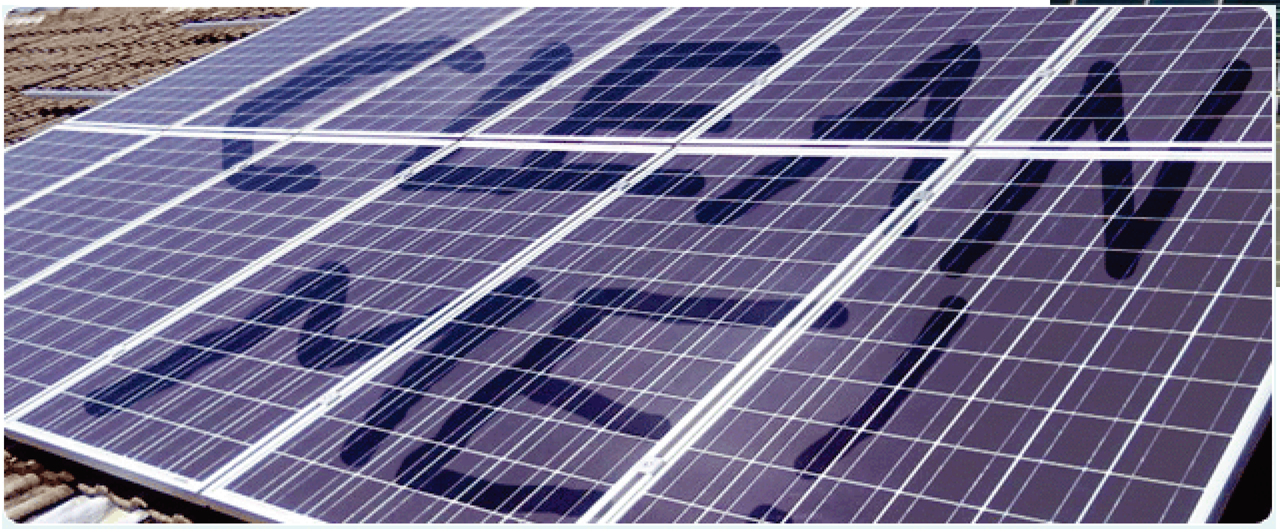
Problem Identification: An example of this toolset…

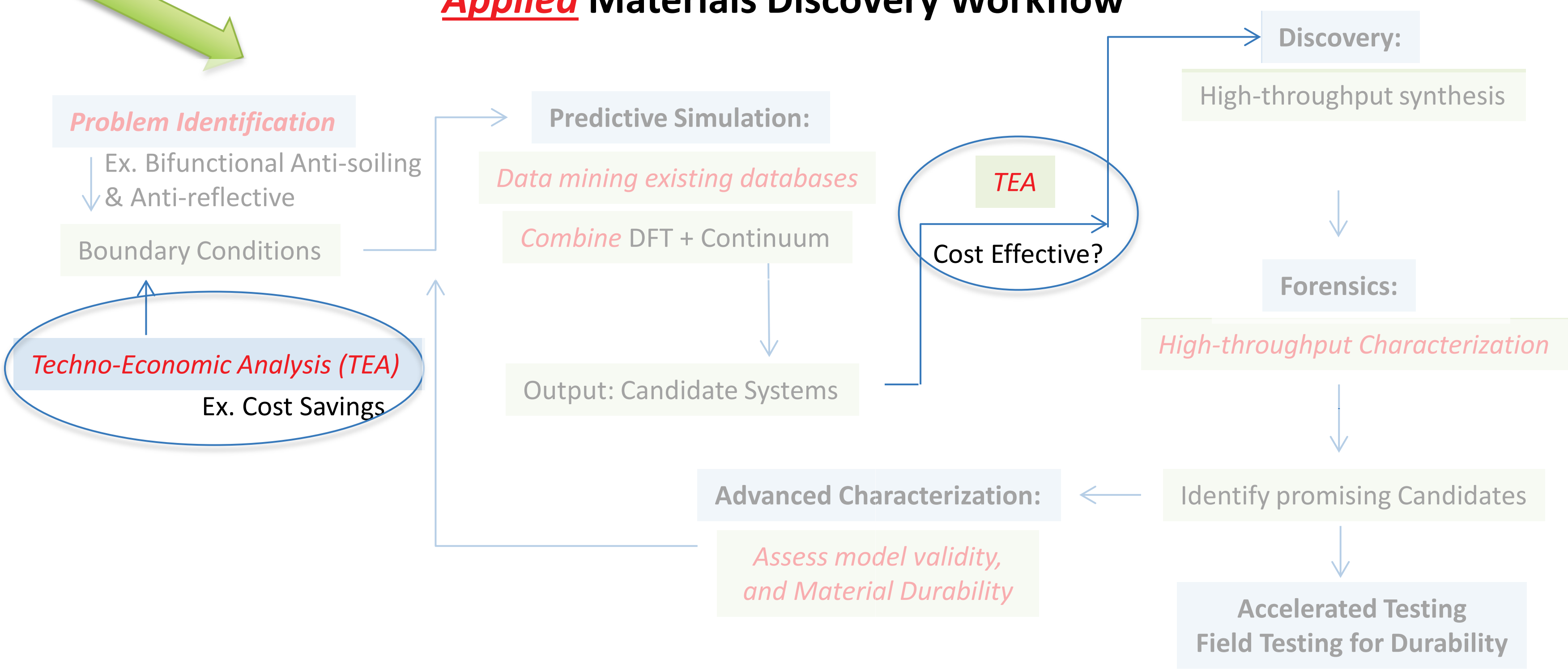
- Dirty panels can result in efficiency loss & can be difficult to clean
- Complex problem: dirt is different everywhere
- Coating durability, and function important

Can our toolset design/develop/screen antisoiling (AS) antireflective (AR) coatings in a rapid, high-throughput manner?



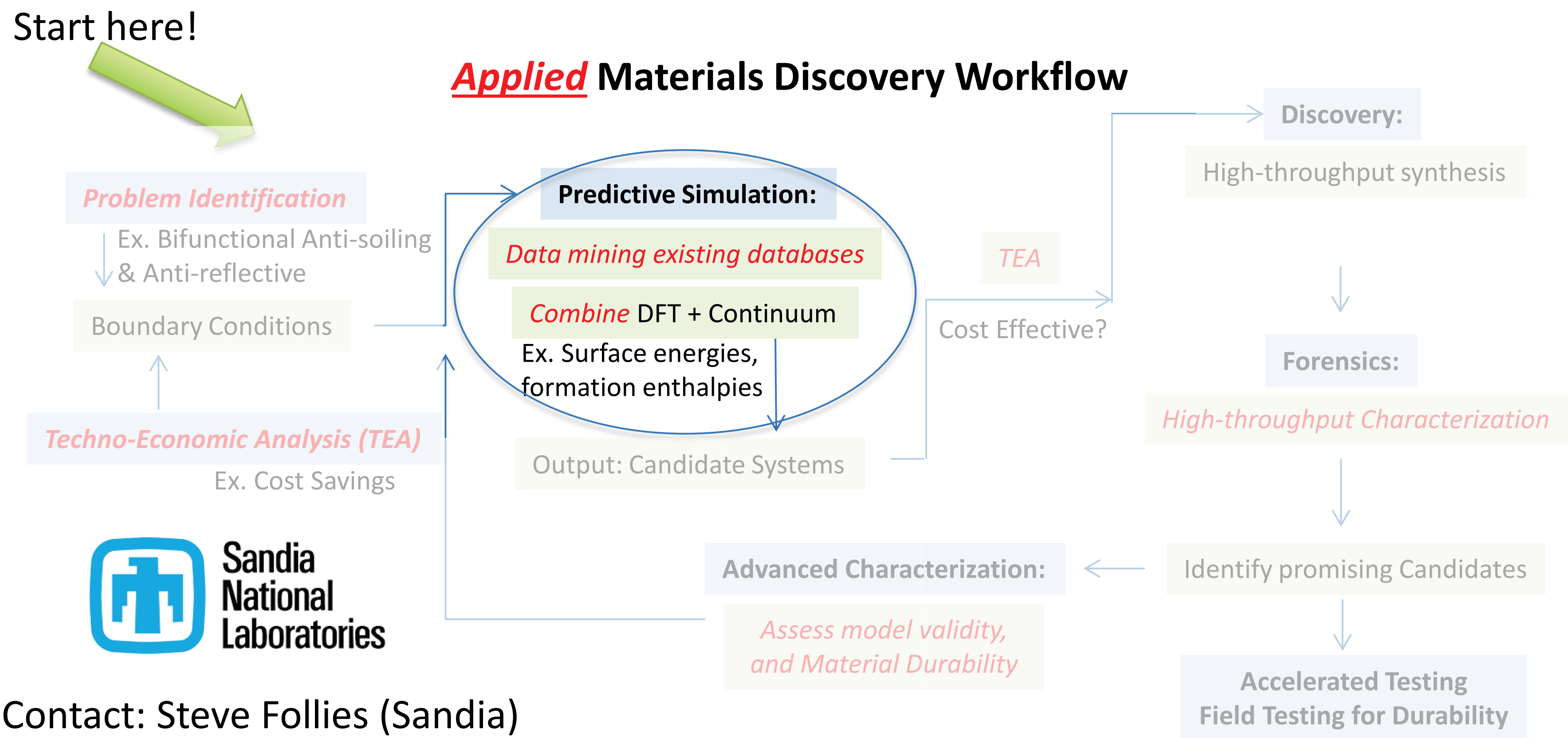
Start here!

Applied Materials Discovery Workflow



Techno-Economic Analysis:

- **Raw material selection, cost effective?**
- **Economic impact**
- **Is the efficiency gained worth the cost of the coating?**
  - **Regional soiling rates**



Contact: Steve Follies (Sandia)

Predictive calculations of surface/interface thermodynamics

Surface fouling: surface and surface/adsorbant interfacial energies

- Contact angles, adhesive energies,

Long-term goal: develop computational methods – applied materials

- thermodynamic quantities
- density function theory (DFT) -> predictive capability

Short-term goal: develop computational/theoretical protocols for surface energy

- model binary → model ternary systems

Data mining with DuraMAT Data Hub

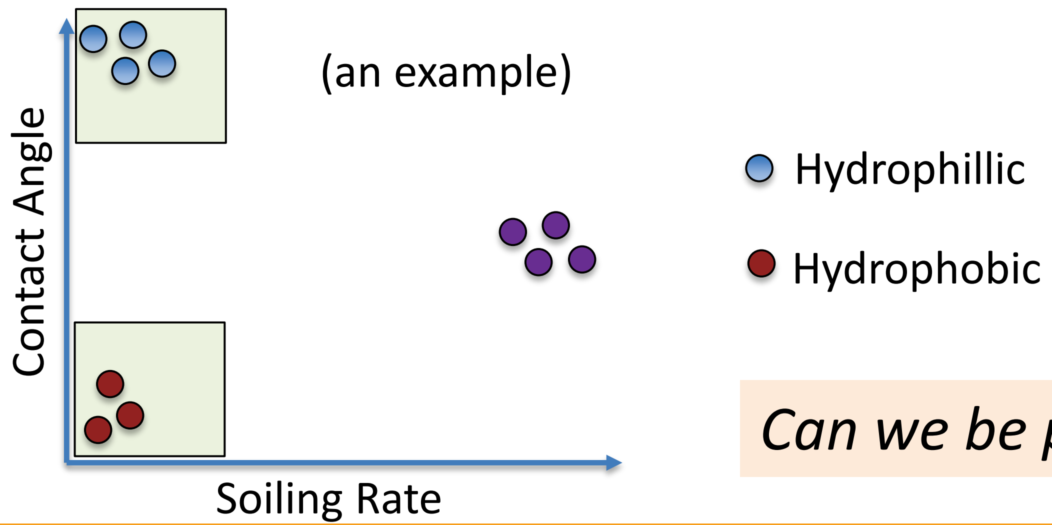
Material descriptors

- Chemical structure = TiO_2, SiO_2
- Morphology = nanoscale roughness
- Layered structure = thickness

Functional Properties

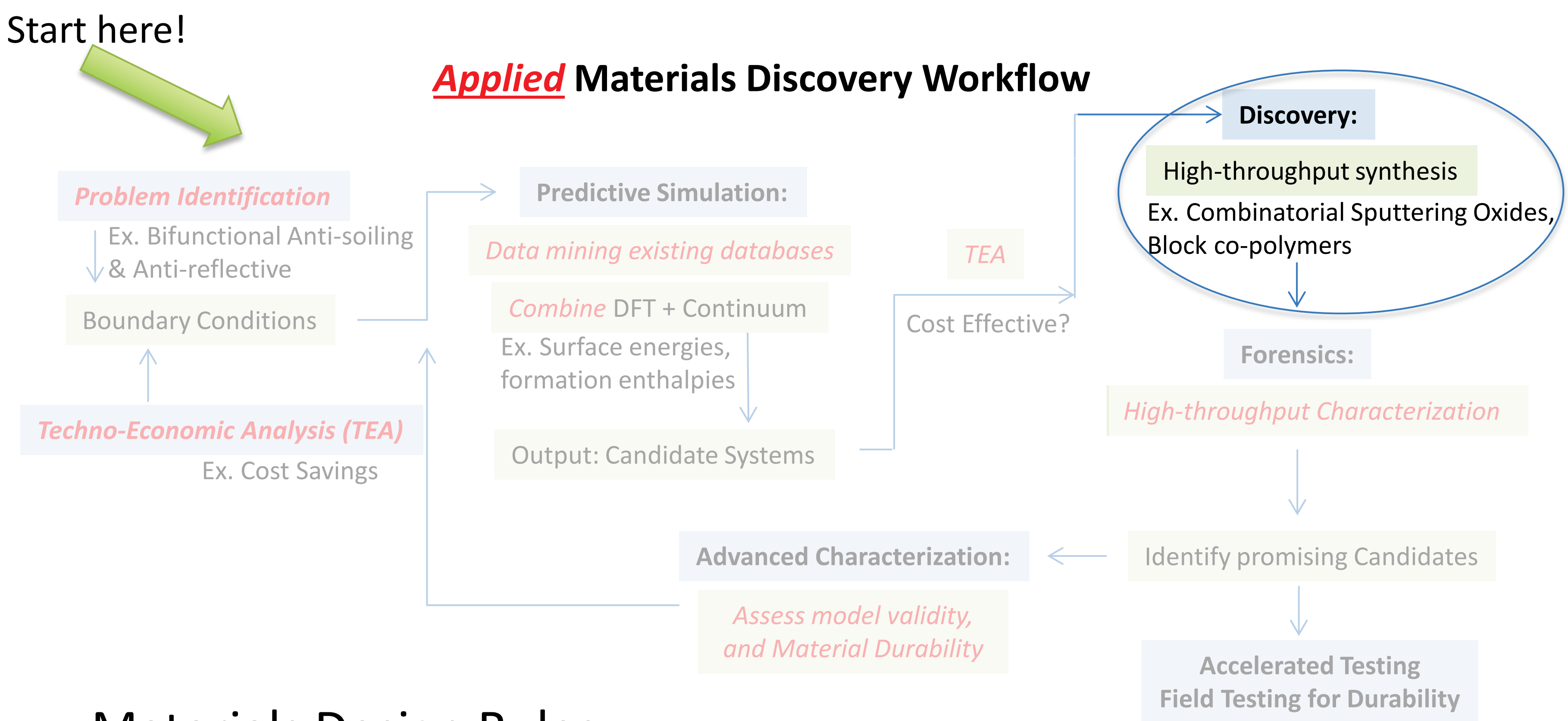
- Contact angle: Hydrophobic/hydrophilic
- Transmittance/reflectance: antireflective
- Surface energy/chemical reactivity : cementation/soiling rate
- Degradation rates

Mine existing literature + patents to build database
Machine learning -> correlation between descriptors & properties



Can we be predictive?

Applied Materials Discovery Workflow



Materials Design Rules:

- Manufacturability
- Compatibility w/ module manufacturing protocols
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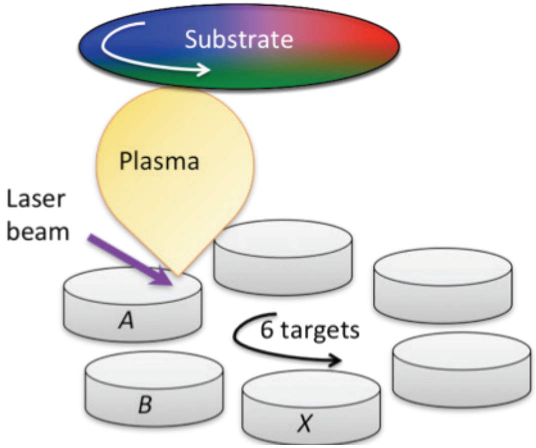
- Optical Properties
- Durability

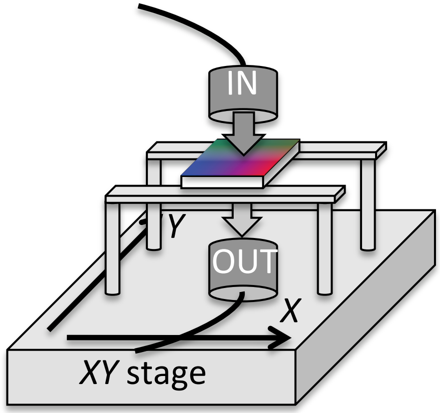
Demonstration of high throughput synthesis and characterization

Combinatorial Pulsed Laser Deposition



- Adopt the existing high throughput thin film deposition
- synthesize libraries of new bifunctional (AR, superhydrophobic) oxide coatings.

Optical Transmittance/Reflectance Mapping



- Upgrade the existing spatially-resolved optical characterization instrument
- enable diffuse transmittance/reflectance measurements

NREL NATIONAL RENEWABLE ENERGY LABORATORY Andriy Zakutayev (NREL), Andriy.Zakutayev@nrel.gov

Digital printing/coating capabilities at the Advanced Materials Lab

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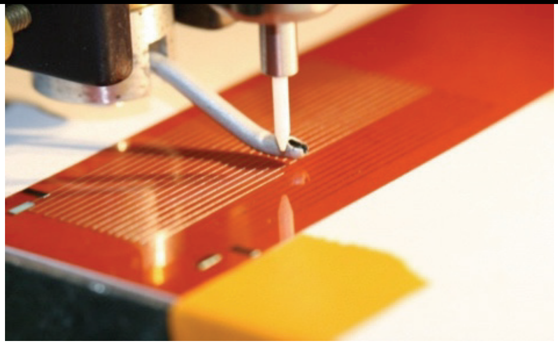
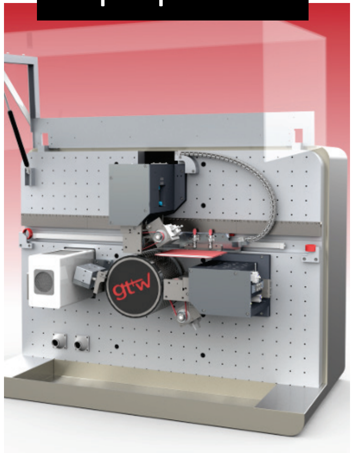
Deposition of soft materials (e.g. block copolymers)

- printing to explore soft materials as AR and AS coatings
- Example: Varying block lengths in block copolymers

Direct-Write by Aerosol and Ink Jet



Superproofer



RK Printers/coaters

Select Current Capabilities:

- Multilayer registration gravure/flexo system
  - <10 µm feature size and registration accuracy (GT+W Superproofer).
  - hard (e.g., Si wafer) & flexible substrates.
- Ultra-fine feature (~150 nm) 3D additive manufacturing system (Nanoscribe)
- Meter bar, flat plate-gravure (RK)
- Direct write: Aerosol, ink jet (2D) and extrusion casting (3D)
- Integrated Nanoink-synthesis and development capability

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Contact: Bryan Kaehr (Sandia), bjkaehr@sandia.gov

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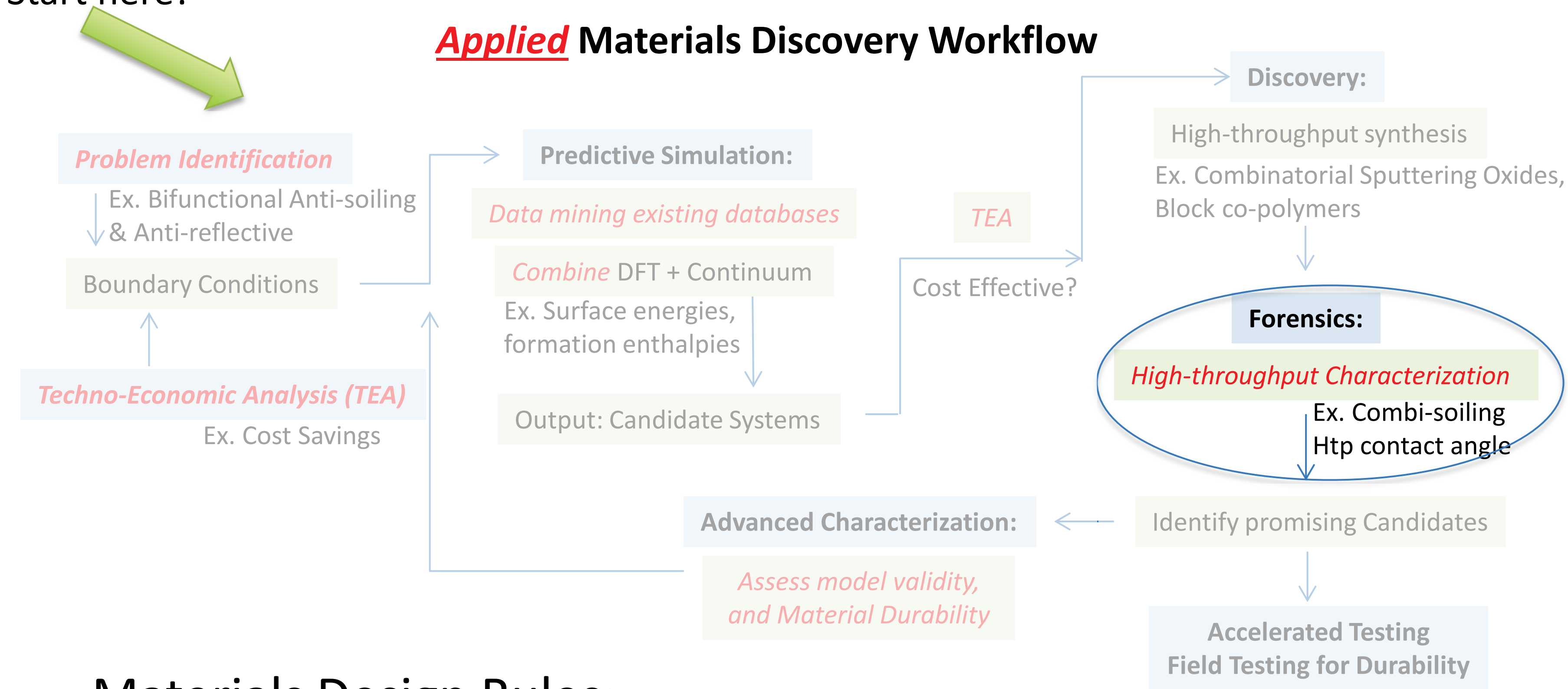

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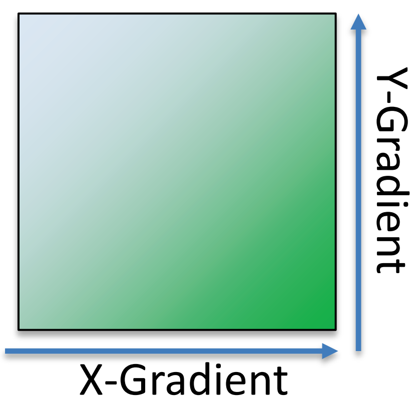

High Throughput Contact Angle Measurements

Upgrade single droplet system to a motorized stage with µm droplet deposition and automated camera.

Will enable:

- Rapid testing of a matrixed surface & multiple samples
- Repeatable and programmable path for droplet deposition
- Precise volume deposition

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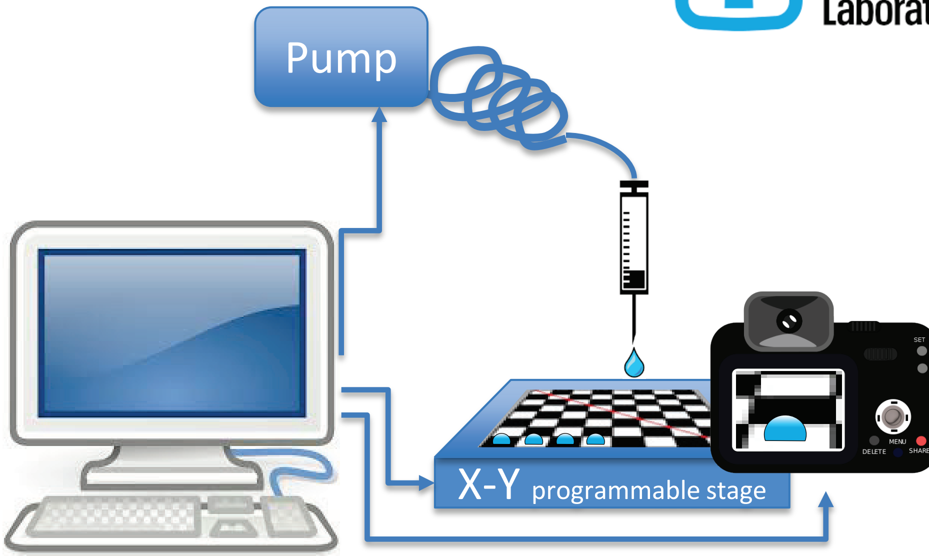

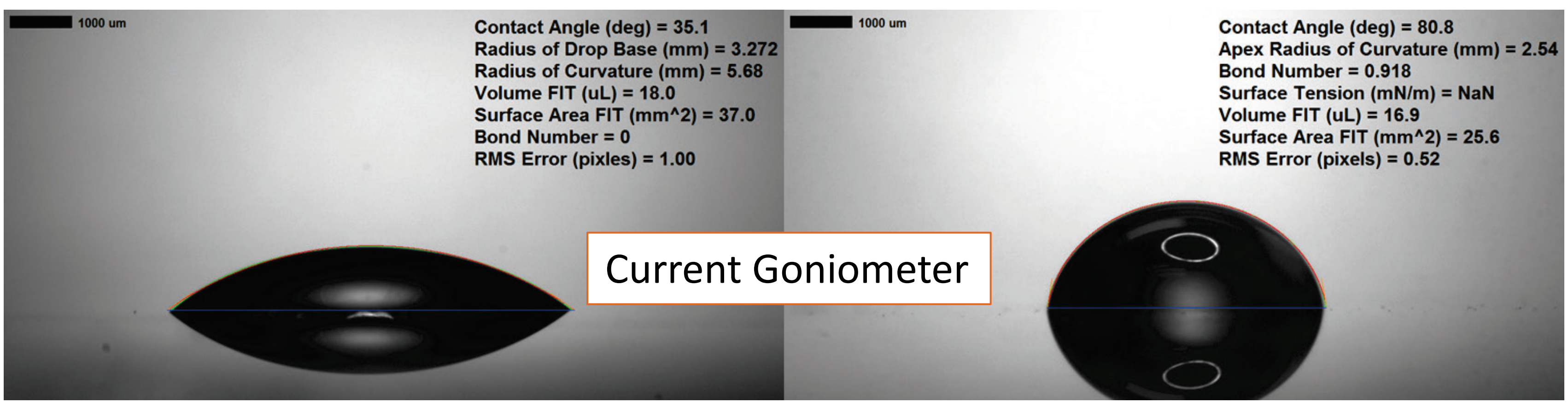

Contact: Margaret Gordon (Sandia)megord@sandia.gov

Combinatorial Artificial Soiling

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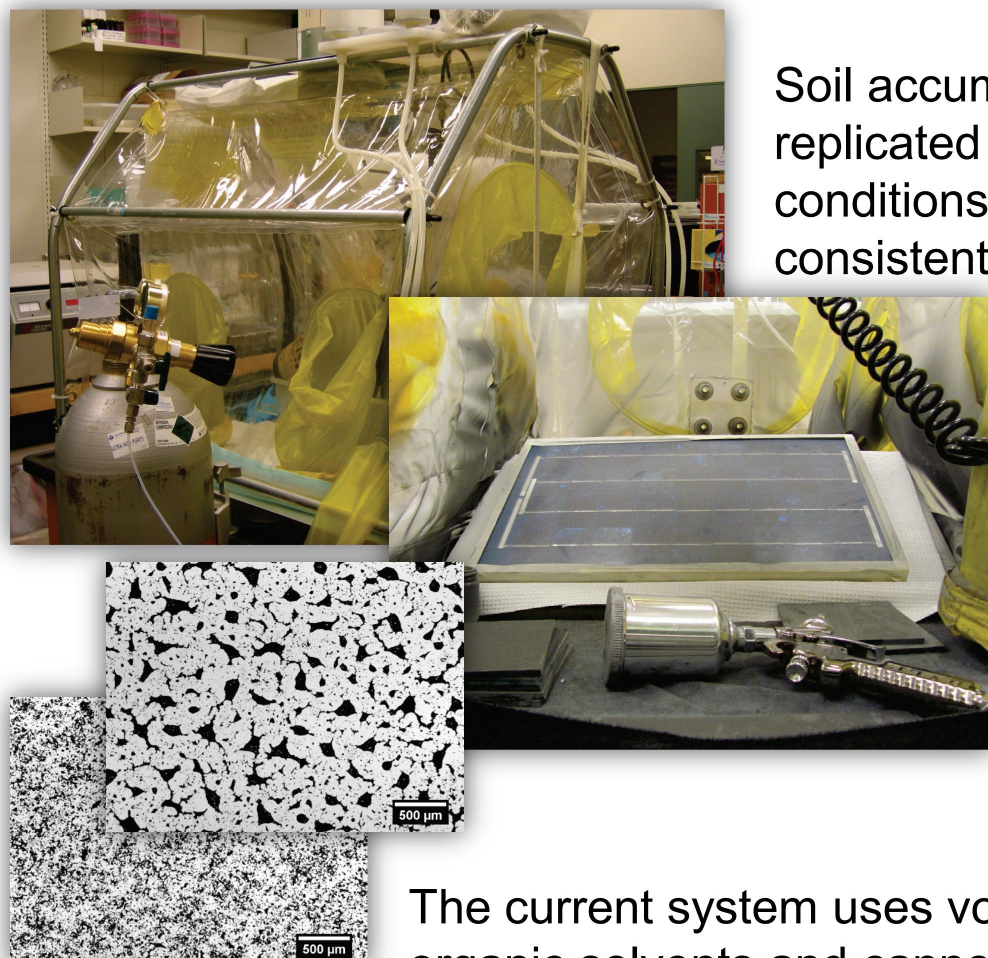
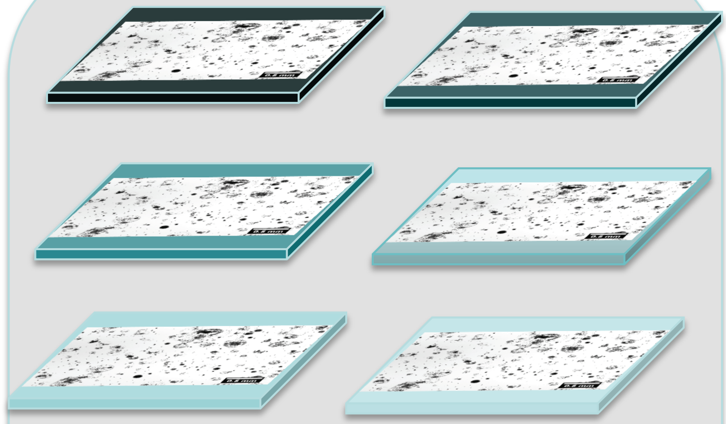


Soil accumulation can be replicated under laboratory conditions to achieve very consistent mass coverage.

The current system uses volatile organic solvents and cannot completely replicate microscopic patterning.



Planned Upgrade:
Adaptation to an aqueous print system will allow the same pattern to be printed on a variety of different surfaces.

Contact: Bruce King (Sandia) bhking@sandia.gov, Patrick Burton (sandia) pdburto@sandia.gov

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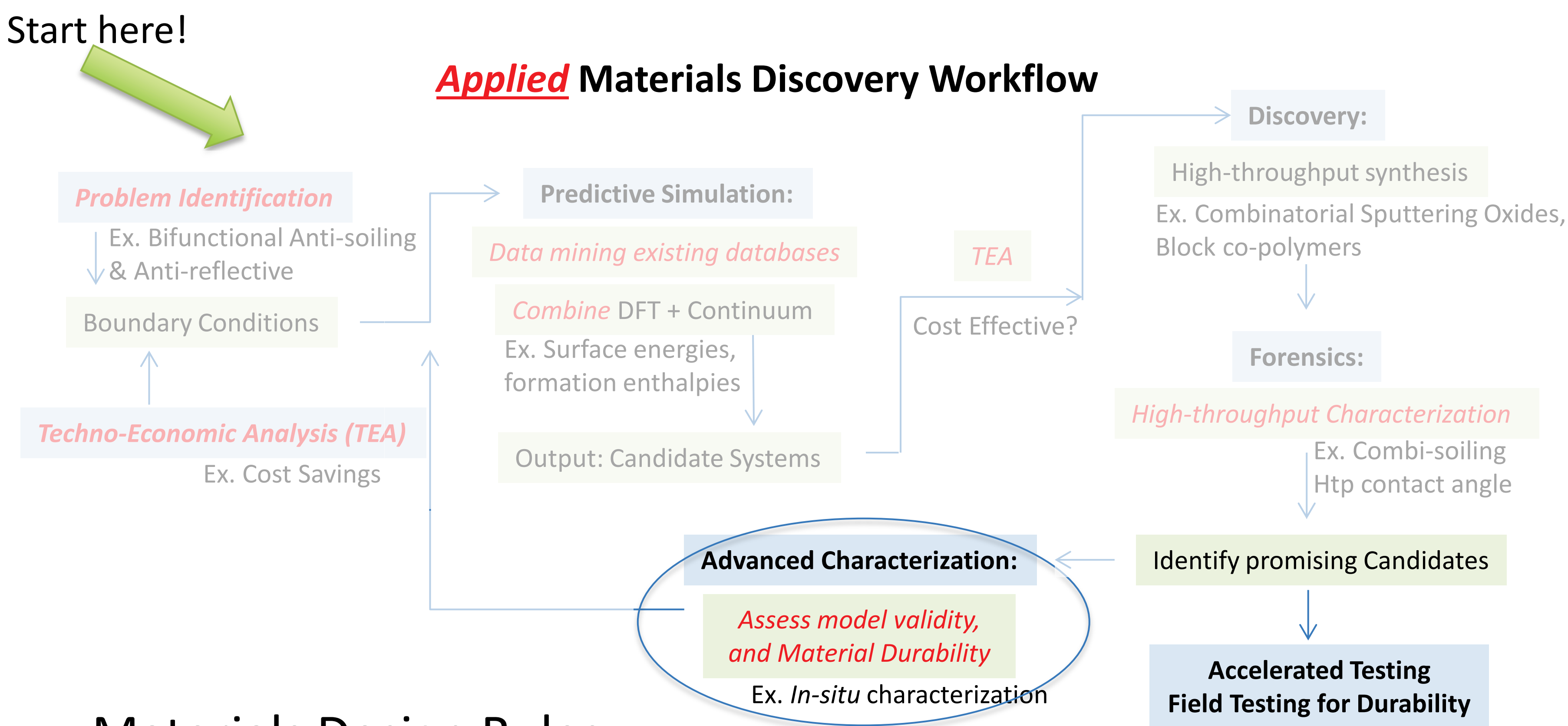

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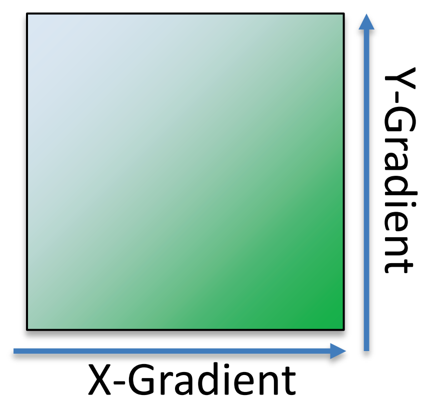

Advanced Characterization:

- **Challenge**: Understanding chemically and morphologically what is happening to coating materials as they age and degrade

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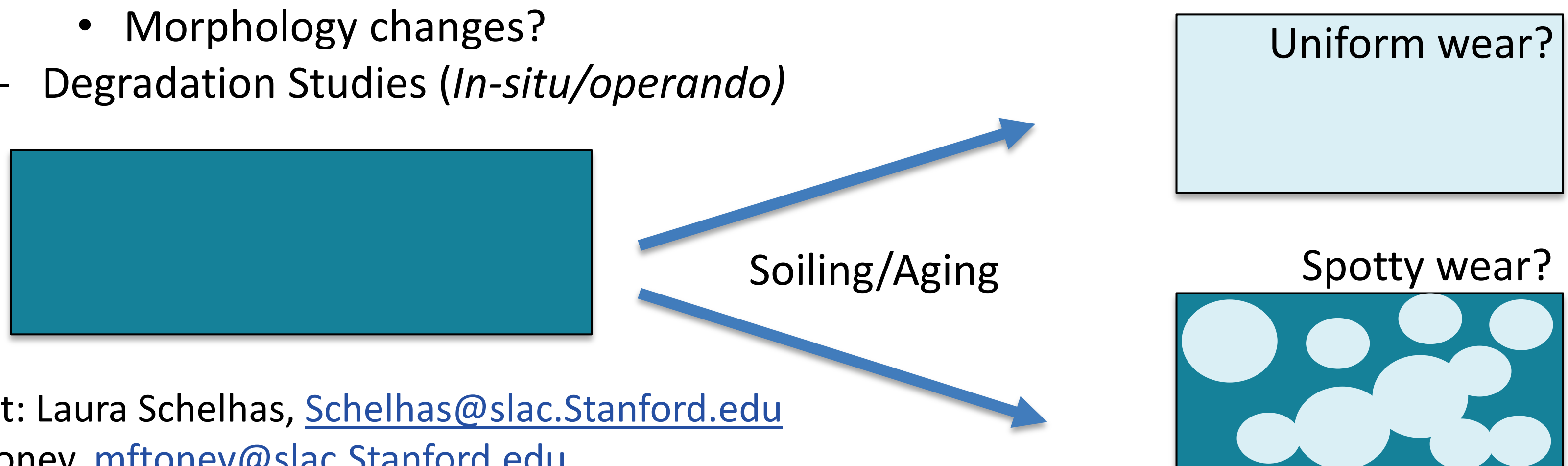
- **Example experimental protocol**:
  - Suite of characterization tools to understand as deposited coating
    - Chemically: scanning Auger, nano-SIMS, x-ray absorption spectroscopy
    - Morphology: porosimetry, SAXS, reflectivity, AFM
  - Soiling/Aging Tests
    - Field testing (Cap 5)
    - High-throughput soiling system
  - Repeat characterization after soiling/aging
    - What changes to the surface chemically?
    - Morphology changes?
  - Degradation Studies (*In-situ/operando)*



Contact: Laura Schelhas, Schelhas@slac.Stanford.edu
Mike Toney, mftoney@slac.Stanford.edu

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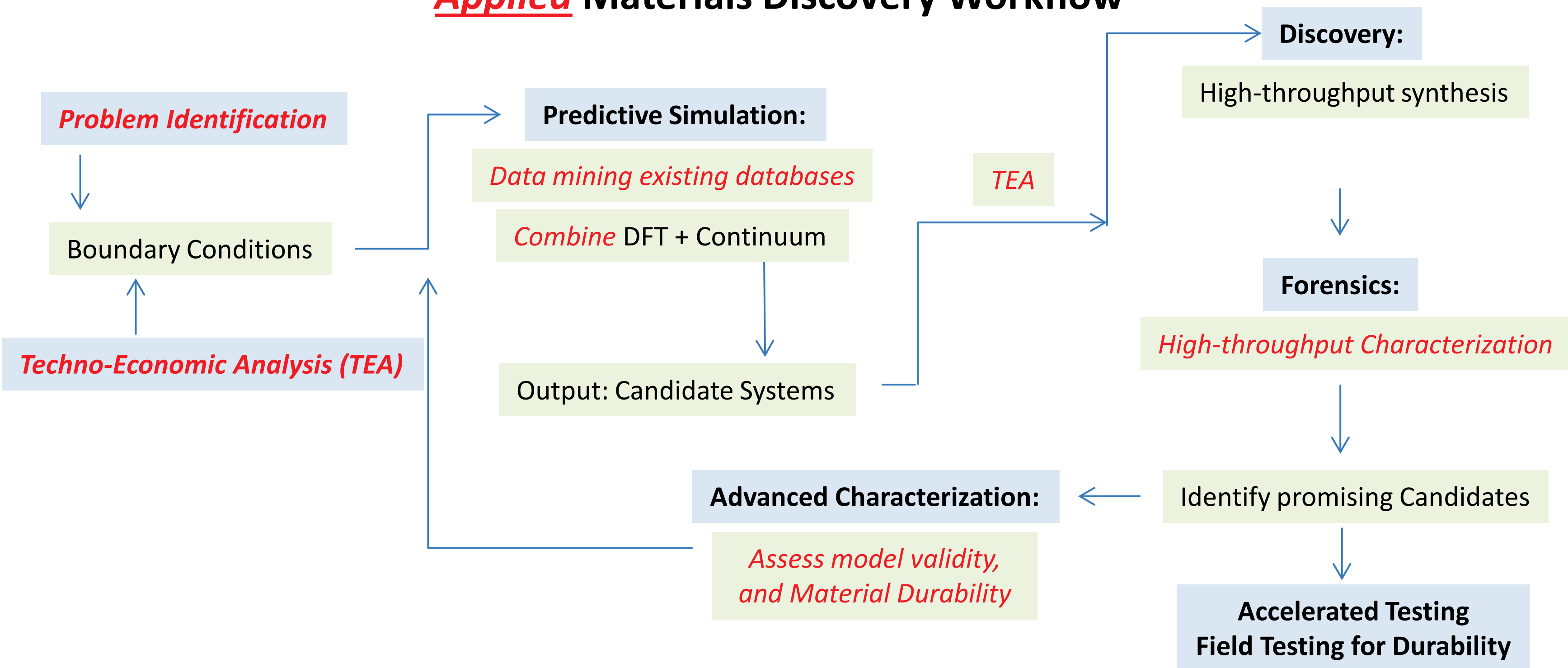

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This is an example of how the Materials Discovery and Forensics tools can be applied to PV challenges. More synthesis/characterization tools are available for collaboration. Please contact our team for further discussion!

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Materials Discovery and Forensics POCs

- **Simulation:**
- Steve Folies (Sandia), foiles@sandia.gov
- **Synthesis:**
- Bryan Kaehr (Sandia), bjkaehr@sandia.gov
- Andriy Zakutayev (NREL), Andriy.Zakutayev@nrel.gov
- **Characterization:**
- Margaret Gordon (Sandia), megord@sandia.gov
- Laura Schelhas (SLAC), Schelhas@slac.Stanford.edu
- Mike Toney (SLAC), mftoney@slac.Stanford.edu

Starting a DuraMAT coatings working group, contact Laura if you are interested