Breakout Session 3

* ***How can computational methods and data and data be used to accelerate the design, synthesis, processing, characterization, fabrication and testing of new materials?***

A list of 10 ideas/tech that NASA should consider for development.

1. Computational component to all materials development projects as part of the team. Make a culture shift. NASA leader.
2. Interactive team between experimentalists and simulation people to identify key problems that can be modeled to advance a key capability. NASA leader.
3. Open access to the data. Computational and experimental data. NASA must have.

* Identify computational tools that we have or that need to be developed or improved for each specific problem. NASA fast follower everywhere except where indicated.
* **Mesoscale dynamics**, from quantum chemistry up to ~ 10^9-10^12 atoms, capability to address a number of critical issues, such as interface coupling and load transfer (which is a bottleneck in CNT, BNNT, graphene assemblies, in fibers, in composites).
* **Process modeling** (is a huge gap)
* **Modeling of multifunctional materials** and loadbearing structures. NASA leader.
* **Physics based tools:** emphasis on multiscale modeling across length and time scales, accelerated dynamics methods.
* **Computationally mapping** “synthesis” routes. If you have a specific material, what is the path to make it.
* Machine learning tools.
* Exploring new materials and microstructures from ab-initio.
* User friendly tools.
* Tools for advanced manufacturing – design and certification;
* Material lifetime prediction tools: accelerated dynamics methods.
* Stochastic models
* Growth mechanisms for nanostructures (CNTs, nanowires, etc.) NASA watcher.
* Nucleation of crack/failure, possibly of melting, possibly of radiation-induced defects, electrical breakdown (down-select/add relevant examples) in extreme conditions.
* Quantifying model **uncertainty. Certification**. Reliability. NASA leader.
* **Virtual characterization** and data analysis & visualization. Digital image analysis. Access to SOA characterization capabilities. NASA fast follower.
* **Aging** and material environmental compatability. NASA leader.
* **Data mining**: data processing and characerization capabilities to guide the design of future materials. Encourage publications. NASA fast follower.
* Data search (Data google). NASA watcher
* Validation and verification. NASA leader/watcher
* Collaborate with other entities – agancies/academics, etc., not to duplicate efforts. NASA fast follower.
* NASA to fund the development creating a material database which includes the specific test data available. NASA leader
* Creating an HPC team at NASA, hiring more people (not just hardware) specifically related to materials science across the centers and sustain that skill. Fund foundational engineering. NASA leader

1. An assesment of NASA’s role – Load – Watch – Follow
2. Report on rationale for Tech Area and Role
3. In report out, comment on integration across new materials, processing innovation, and computational acceleration.

Technology leader role: NASA develops and demonstrates

Fast follower role: NASA rapidly adopts, accelerates

Technology watcher role: NASA uses the leverage

2 hour block for brainstorming

1 hour deriving the list of top 10 ideas/concepts /tech areas

1 hour define NASA role.