

## **Technology/Capability Overviev**

- Traditionally, the field of materials science has predominantly focused on processing establishing structure-property relations, a material properties. This empirical approace shifting towards the design of materials to functionality, resulting in a paradigm shift research and development from experiment knowledge creation to integrated computat and experimental-validation approaches.
- Current computational capabilities based of calculations and computational modeling e systematic and efficient search of optimal of chemistry and processing parameters for

## Industry Significance

- Adjust processing parameters with respect of materials chemistry in batches
- Confine chemistry specifications of materia improvement of processing robustness
- Develop new materials and processing rout



# **NETL-RUA** Computational Approaches for Materials Design

W	Benef
e and engineering g materials, and measuring	• Dat ma
ach is increasingly o achieve optimal in materials ental based ational-prediction	• Use sta ma
	Oppol
on first-principles enable more combinations	• Dev and
for alloy design.	• Col aut
ct to variations	Devel
	• Dis as s
ials for	
outes efficiently	Conta
	Prof.
	201 S (814)

#### fits to Partner

atabases and database management for specific aterials and their applications for process design

sed by companies and institutions globally in various ages of materials research, development, and anufacturing

## rtunity

evelopment of solutions for design, development, nd processing of materials of interest

Ilaboration on development of a database tomation system

#### **Iopment Status**

stributed depending on specific applications shown in the Industry Significance

#### act

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