

# Computational techniques for materials-by-design<sup>1</sup>

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This presentation will briefly review a number of innovative computational techniques that are being developed in our laboratory towards materials-by-design. Topics to be discussed include multiscale modeling and design in material processes (deformation and solidification), microstructure model reduction, statistical techniques for exploring process/property/structure maps in materials and information-theoretic models for uncertainty propagation in materials modeling and design. We will conclude with a discussion on the development of efficient ab initio-based multi-body energy expansions for property and phase structure prediction of alloys with application to adsorption processes.

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<sup>1</sup> Invited presentation at the GE Global Research Center, Niskayana, NY, March 22<sup>nd</sup>, 2007.