IT-001 **<Invited Speaker>**

Atomic-Scale Insights into Material Properties and Design

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This presentation will focus on computational materials research carried out across length scales. Examples will be presented that illustrate the way in which state-of-the-art quantum mechanical calculations and atomistic simulations can be applied to explain experimental data, design new structures, determine mechanisms, and enable new investigations. In particular, the presentation will present key findings from an integrated experimental and computational investigation of the tribological properties of polytetrafluoroethylene and its composites and predictions regarding the mechanical and tribological properties of inorganic nanostructured materials.