Md Shahrier Hasan

Graduate Student, University of California San Diego

Multi-scale Modeling of the Mechanical Properties of the Nano- structured Materials

- The goal of the research project is to develop computational methods to model the mechanical properties and apply them to understand the mechanisms of deformation behavior in nanostructured materials.
- This involves molecular dynamics to describe dislocation interactions with grain boundaries and interfaces at the atomic and nanoscale.
- Atomistic to Continuum Finite Element Coupling to understand dislocation motion at the microscale

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The key takeaways from SI2019:

- For Molecular Dynamics Simulation, optimize the size of the atomic system that can be modeled with effective parallelization for the available computational resource of the project
- Coupling with a suitable Continuum Finite Element software to implement Concurrent Multi-scale Modeling technique
- Effective visualization approaches to track atomic data