MAterials Genome Innovation for Computational Software

Software & Data Sharing

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Software Distribution & Community Code Development

- **Software distribution**: Open-source software for computational synthesis & diagnosis will be distributed to the community on Github.
- **Community code development**: Workshops will be organized to train users & interface with the scientific community of software developers.
MAGICS Software

Singh group
• Thermal transport plug-in

Prezhdo group
• Nonadiabatic quantum molecular dynamics (NAQMD) plug-ins
  > Surface hopping with decoherence
  > Multi-electron processes

Goddard group
• ReaxPQ
• aARRDyn

Vashishta, Kalia, Nakano
• Scalable molecular-dynamics (MD) engines: DCR-QMD, XRMD
• Computational synthesis (exfoliation & iCVD) plug-ins

DCR: Divide-conquer-recombine
QMD: Quantum molecular dynamics
XRMD: Extended Lagrangian reactive molecular dynamics
iCVD: Initiated chemical vapor deposition
MAGICS Data

• Disseminate simulation & experimental data produced by the Center through the LBNL Materials Project & USC Center for High Performance Computing

• Devote apps on the Materials Project for data-mining aggregate data & searching for optimal synthesis conditions, given a target material

• Employ the Materials API to encourage external collaborators to independently extend the analyses & make the results available to the community