

Analysis of Thermal Transport in Graphite Intercalated Compounds

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Purpose	Uncover the mechanisms observed in GICs experiments.
Outline	NEMD Simulation of FeCl ₃ -GIC system
Result	Suppression and Control of Thermal Transport

Computing system:
node-hour
Software
parallelize

SQUID General Purpose CPU nodes
35 node-hour
LAMMPS
152 nodes

