 ICCES, vol.13, no.3, pp.63-63

Hybrid Quantum/Classical Approaches of Nano- and Meta-Materials

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Summary

Unique properties in artificially designed new materials are demonstrated via multiple-scale computational techniques. A density-functional/classical molecular-dynamics method is employed to investigate segregation dynamics of dopants in nanostructured ceramics/semiconductors. We also develop a classical electromagnetic simulation algorithm combining with an electronic-structure calculation for analysis on optical properties of meta-materials. We demonstrate that these novel algorithms are highly optimized for ultra-scale parallel computers.

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