

Quantum Mechanical Algorithm for Large-Scale Simulation of Materials

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The computational study of formation and rupture of chemical bonds amongst atoms in materials at various temperatures and pressures requires an algorithm based on quantum mechanics. Our objective is to implement a quantum mechanical procedure able to treat an unprecedentedly large number of atoms in realistic first-principles computational studies of materials relevant to the Laboratory's mission.

Conventional implementations of quantum mechanical approaches to materials science suffer from a severe computational obstruction that impedes their use in large scale simulation because their computational cost scales as N^3 , or at best N^2 , where N is the number of atoms included in the calculation. Our novel approach differs radically from conventional implementations in that it is computationally much more efficient because its

computational cost scales only linearly with the number of atoms while at the same time retaining the same accuracy of the older conventional implementations.

For any given Hamiltonian matrix H , our method finds the ground state energy E by calculating the electron density matrix ρ that minimizes

$$E = \text{Tr}(H\rho)$$

subject to the constraints

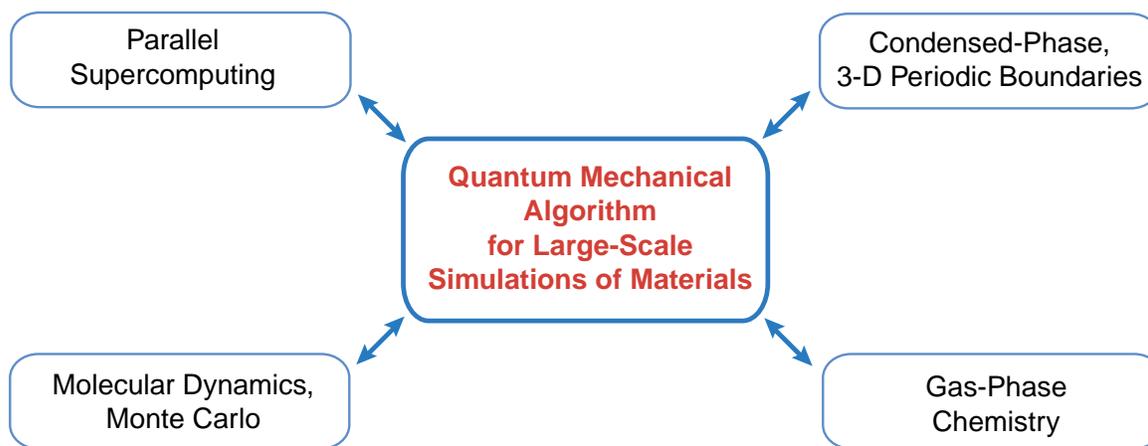
$$\rho = \rho^2$$

and

$$\text{Tr}(\rho) = n$$

where n is the number of electrons.

The figure illustrates directions for expansion of our method into an extremely powerful tool for computational studies in the field of materials science.



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