“Truly Scalable O(N) Approach for First-Principles Molecular Dynamics of Non-Metallic Systems”

Jean-Luc Fattebert

We present a scalable O(N) First Principles Molecular Dynamics algorithm based on a non-orthogonal localized orbitals formulation of Density Functional Theory. A scalable strategy is used to approximately compute selected elements of the inverse of the associated overlap matrix. The algorithm, which exploits sparsity and uses nearest neighbor communication only, shows excellent scalability. Accuracy is controlled by the mesh spacing of the finite difference discretization, the size of the localization regions confining the orbitals, and a cutoff radius for the overlap matrix.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.