Nano-material tools/ codes on nanoHUB

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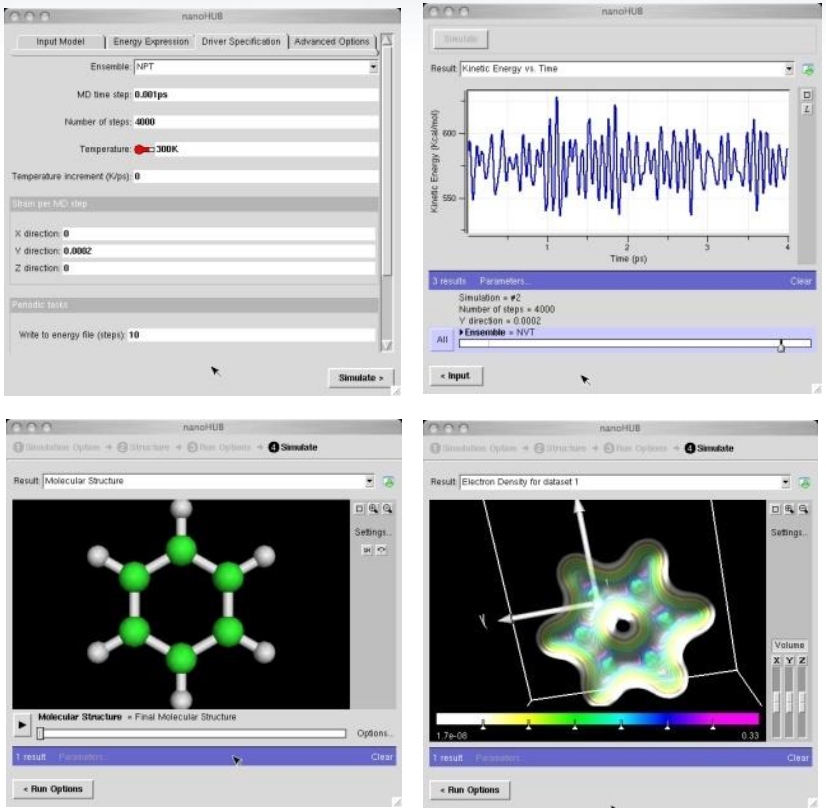
Objective: Deploy educational and research tools for electronic structure simulations and molecular dynamics of nano-material on nanoHUB



Method:

- Write programs/ Tcl scripts
- Use knowledge of DFT and MD and exisiting codes, prepare examples
- Use rappture interface

Results:

- MATLAB code for Hartree Fock calculations of H_2 molecule
- nanoMaterials Simulation Toolkit with GUI for MD and DFT simulations
- ABINIT on nanoHUB for DFT with GUI

Impact: The tools/ codes have already served more than 4000 users