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EXPLOITING GRID FOR CONDENSED MATTER APPLICATIONS: QUANTUM DOTS AND BUILDING CLUSTERS ATOM-BY-ATOM

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QUANTUM DOTS: A fully self consistent real space DFT approach has been implemented.
We calculate the ground state charge and spin density, magnetic state, eigenvalue spectrum and investigate effects of impurity over a wide range of sizes of quantum dots (50-300 nm with 2-20 electrons). The results reveal Wigner localized state (Wigner molecule). The impurity induces the novel magnetic states ans anti ferromagnetic spin distribution and enhances the localization.
CLUSTERS: We have obtained equilibrium geometries (~100) of clusters of Sodium (Sizes 20-150) by a combinations of simulated annealing and local minimization. We calculate stability, binding energies, HOMO-LUMO gap etc. We also investigate growth patterns and fine that the growth shows order- disorder cycles. The shape analysis of the ground states is shown to be correlated with the shapes of heat capacities. Thus nature of the ground states and the isomers spectrum dictates the behavior of clusters at finite temperature.

3. Impact

For both the problems the possible SCF solution need several hundred independent runs which can be executed asynchronously. In the first problem, for a fixed value of dot size ~100 SCF runs are needed (for fixed number of electrons). A exhaustive study of up to 20 electron QD, needs in the few hundreds of thousands of runs. Although the single run of this calculation is not CPU extensive, the mare number itself is too heavy for a small cluster to perform the calculations in reasonable amount of time. Similarly for the finding isomers of a single cluster typically 400 minimization are executed.The number of jobs to be executed turns out to be number of clusters*400*charge state. For a thorough understanding of evolutionary characteristic we undertake 3 types of clusters: Na_n (Jellium, n=20-147), Ga_n (covalent n=20-70) and Al_n (n=20-70). The magnitude of the computational intensity can be guessed from the fact that the total no of runs required is ~100,000 (~5 Hrs per run).

URL for further information:

http://physics.unipune.ernet.in/~cmg/grid.html

4. Conclusions / Future plans

For a class of problems discussed here the grid computing turns out to be extremely efficient. (Resources: EGEE,Garuda,Local machines) The number of runs required are ~100000 and each can be executed on P4, Xeon machines. We have obtained the results ~50 clusters of Na (with shoot-and-forget strategy). Future plans involve Na_n (n=20-147) and Ga_n(n=20-70). The resulting detailed comparison of the growth pattern is expected to answer a fundamental question: “how do clusters grow, atom by atom?”

Provide a set of generic keywords that define your contribution (e.g. Data Management, Workflows, High Energy Physics)

Quantum dots, Impurities, Wigner, Atomic Clusters, Electronic Structure, Density Functional Theory

1. Short overview

Quantum Dots (QD) and clusters represent novel nanostructures with applications in semiconductor electronics, organic dyes, catalysis etc. Their electronic structure is crucial for tailoring desired properties. We use grid to calculate their properties (band gaps, bonding, stability, magnetics state, quantum states) using

self consistent field (SCF), density functional theory (DFT). We also investigate evolution of properties as a function of size. The work is done under EU-India grid Project.

Primary authors: Mr PUJARI, Bhalchandra (Pune University); Prof. KANHERE, Dilip (Pune University); Dr JOSHI, Kavita (Pune University); Mr GHAZI, Mohammad (Pune University); Mr ZORRIASATEIN, Shahab (Pune University); Mr KAWARE, Vaibhav (Pune University)

Presenter: Mr PUJARI, Bhalchandra (Pune University)

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