

Eigenvalue solvers for computer simulations of efficient solar cell materials



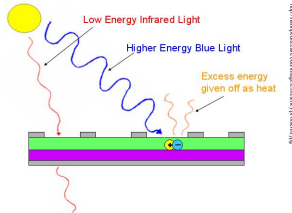
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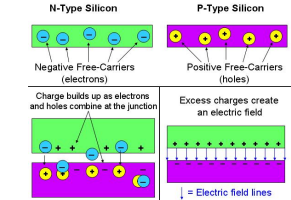


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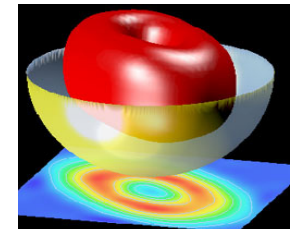
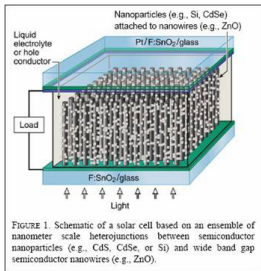
Developing New Efficient Solar Cell Materials



Low-energy light doesn't have the energy required to release electrons; too-high energy light wastes the energy as heat.

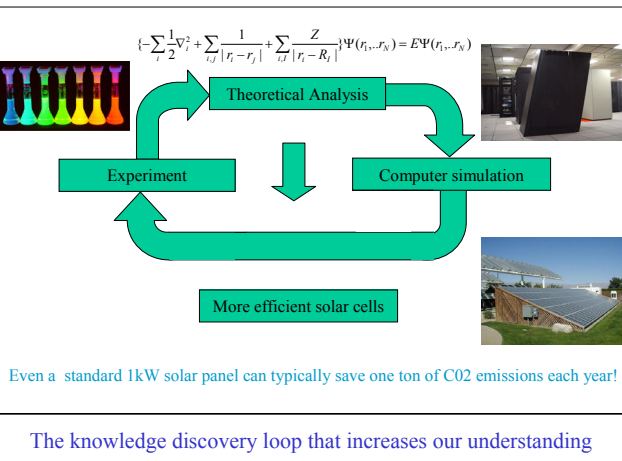


In a standard solar cell, a collision of a photon with the cell material typically results in only one electron to produce electric current.



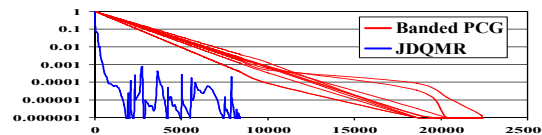
Wave function squared (red) of a hole state in a spherical CdSe colloidal quantum dot.

Several nanosystems, specifically some nanocrystals and quantum dots, have been recently developed and analyzed. They can generate multiple excitons per photon, and thus can potentially increase the solar cell efficiency several times.

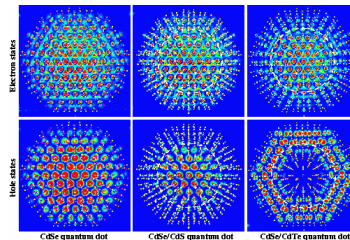


Computational and Mathematical Challenges

Understanding the photo-conversion process in a wide variety of material systems often requires large scale computer simulations based on first-principles theories. Material systems of practical interest have large sizes, which makes their computer simulations difficult. A typical practical simulation may take days, even on the best available supercomputers with thousands of processors. The long simulation time becomes a bottleneck for progress in understanding and developing photovoltaic semiconductors and semiconductor nanostructures for solar panels. Most of the computational time is often spent on eigenvalue solvers.



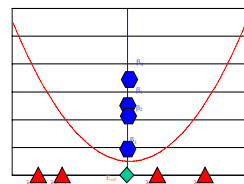
An example of a challenging computation with the PESCAN code (Lin-Wang Wang, NERSC LBL, Computational Research Division): Computing 10 eigenstates of a quantum dot made of 534 Cadmium atoms and 527 Selenium atoms on 16 processors of an IBM-SP. The resulting matrix is dense of order 141,625. We plot the error versus the number of matrix vector products for two different eigenvalues solvers and observe significant acceleration.



CBM and VBM states of pure CdSe, CdSe/CdS and CdSe/CdTe core/shell structure quantum dots (Lin-Wang Wang, NERSC LBL, Computational Research Division.) These six figures represent eigenfunctions and have required several hours of computational time on a large machine with the PESCAN code. Speeding up the eigensolvers accelerates the whole scientific discovery process.

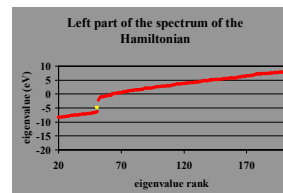
Interior Eigenvalue Problems

In some situations, the energies (eigenvalues) of interest are interior eigenvalues around the band gap. (Yellow in the right-hand side Figure). They correspond to the CBM (conduction band) and VBM (valence band). Most of the observable physical properties depend on those energies.



Interior eigenvalues are harder to compute than the extreme ones. Current techniques rely on spectral transformations, e.g., the Folded Spectrum Method, where the Hamiltonian operator H is transformed into $(H - E_{ref})^2$. The left-hand side picture illustrates the effect of the spectral transformation on the eigenvalues. Instead of seeking λ_3 , which is an interior eigenvalue, we are seeking β_3 a minimum eigenvalue.

$$T(A - B)x = 0$$

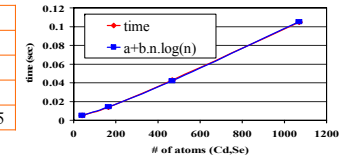


Preliminary Results on Numerical Scalability in PESCAN

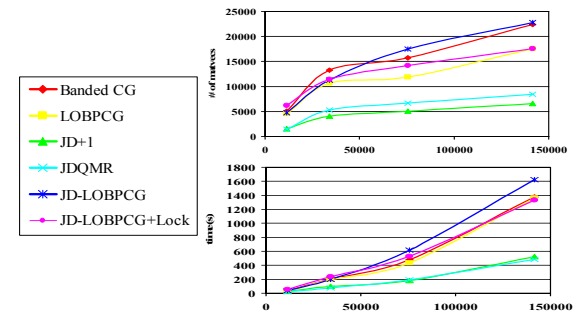
A sample of increasing size quantum dots

	# atoms	n
Cd20.Se19	39	11,331
Cd83.Se81	164	34,143
Cd232.Se235	467	75,645
Cd534.Se527	1061	141,625

Scalability of matrix vector products



We report preliminary results of scalability tests for simulation of a sample of quantum dots with increasing number of atoms and, thus, the problem size. The matrix-vector product operations scale reasonably well, as $n \log(n)$, when the problem size n increases, see the figure above. On the figures below, the number of iterations of Banded PCG does not scale well: when $n=11,331$ grows to $n=141,625$ the number of atoms is multiplied by 12, but the solution time with Banded PCG is multiplied by 33. In JDQMR, the solution time is multiplied by 17, which is an improvement, but still not the ideal scaling.



Scalability analysis in matrix-vector products and in time with respect to the problem size for six different methods using the PESCAN code.

Eigensolvers Software Development Experience for Nanosciences

Andrew Knyazev is the inventor of the Locally Optimal Block Preconditioned Conjugate Gradient (LOBPCG) method and the main developer of the Block Locally Optimal Preconditioned Eigenvalue Solvers (BLOPEX) package. BLOPEX is a general purpose software library that implements the LOBPCG method and is suitable for sequential, shared memory or parallel distributed computers. Interface to widely used packages, PETSc, HYPRE, and MATLAB are available. The LOBPCG method is implemented in one of the most popular nanoscience computation software ABINIT. Julien Langou has added the LOBPCG method and several other eigenvalue solvers to PESCAN, and participated in the software testing and in obtaining results that we report here.

- [1] I. Lashuk, M. Argentati, E. Ovchinnikov and A. Knyazev, Preconditioned Eigensolver LOBPCG in hypre and PETSc. In *Lecture Notes in Computational Science and Engineering*, Springer, 55(2006), pp. 629-637. ISBN: 3-540-34468-3.
- [2] S. Tomov, J. Langou, A. Canning, L.-W. Wang, and J. Dongarra. Conjugate-gradient eigenvalue solvers in computing electronic properties of nanostructure architectures. To appear in *International Journal of Computational Science and Engineering*

Mission objective and statement

Andrew Knyazev and Julien Langou of the Department of Mathematical Sciences at UC DHSC Downtown Denver Campus are looking for a fruitful collaboration with NREL scientists on designing novel eigenvalue solvers specifically tailored for material sciences in order to accelerate and improve nanostructure computations, and to contribute to numerical simulation and development of efficient solar cells.