U.S. Department of Energy
Energy Efficiency and Renewable Energy
Bringing you a prosperous future where energy is clean, abundant, reliable, and affordable

DOE Solar Energy Technologies Program Peer Review

Technical Track: Nano Technology/Materials & Quantum Dots
Project Name: Theory & Computational Science
Principal Investigator: Steven Hammond

Denver, Colorado
March 9-10, 2009

This presentation does not contain any proprietary or confidential information.

Agreement Scope

- Integrate three unique cross-cutting NREL capabilities to build an essential knowledge base for the Solar Program; establish a strong link between theory and experiment
- Theory of Transparent Conductors
- PV Material Theory
- Scientific Data Management and Mining
- Focus on improved understanding of existing materials, develop novel materials, and accelerate the process of moving technologies from theoretical or early stage research into applied technologies
- Address barriers still facing existing PV technologies
- Represent recognition of the critical role that modeling, numerical simulation, and scientific data management and mining play in the research and development process.

Quality, Productivity, Accomplishment

Highlight your team's qualifications

Task led by Alex Zunger and NREL's Solid State Theory Team

Special Recognitions: Invited conference contributions

- S. Lany: Gordon Research Conference on Defects in Semiconductors, Aug 2008
- S. Lany: 2nd International Symposium on Transparent Conductive Oxides, Oct. 2008
- A. Zunger: 2nd International Symposium on Transparent Conductive Oxides, Oct. 2008
- A. Zunger: European MRS Invited Talk; US MRS Invited Talk

Accomplishments

- Comprehensive assessment of the theoretical methods used for the defect calculations in photovoltaic materials--**Significance**: Quality check for theory-predictions
- Identified point defects in $Cu(In,Ga)Se_2$ absorbers that act to limit the solar cell open-circuit voltage--**Significance**: Understanding limitations of current technologies
- Developed and applied methods to predict difficult systems: wide-gap oxides, transition metal dopants, acceptors in oxides. **Significance**--Build capabilities for prediction of p-type TCO
- Completed simulation of TM dopants in ZnO and In_2O_3. **Significance**--New dopants.

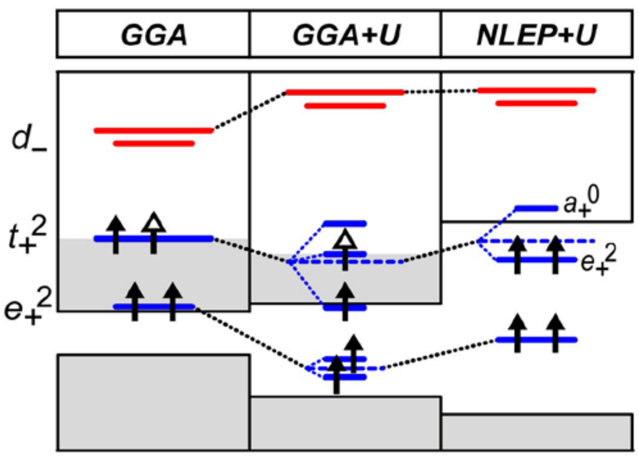
Budget:

- $400K in FY08; $250K in FY09 (CR)

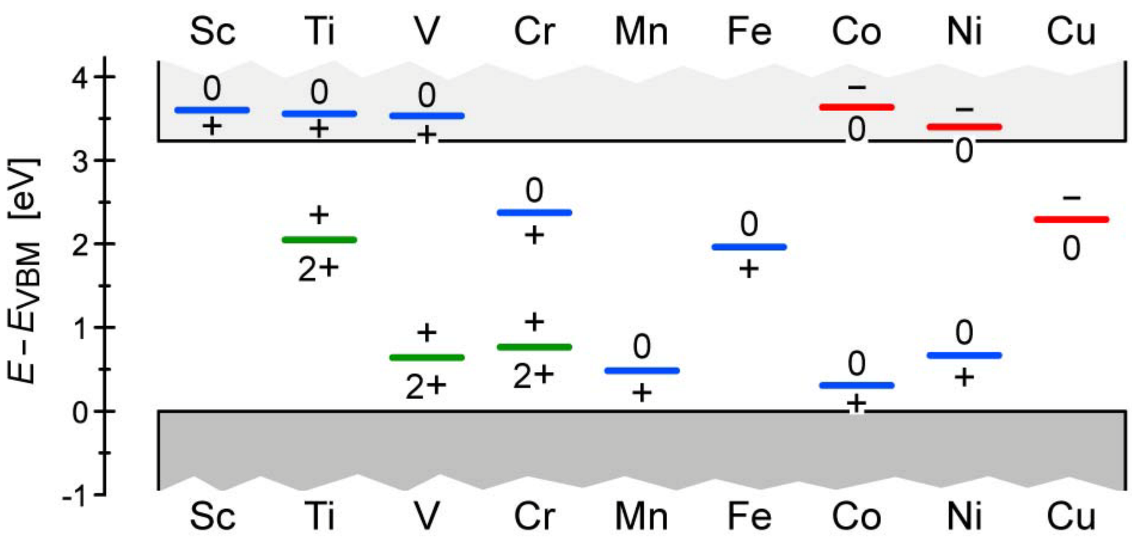
- **Recent experimental work highlights potential of "non-conventional" TCO involving transition metals (TM): TiO_2:Nb, ZnO:V**
- **Prediction of electronic levels of TM requires highly non-standard methods**

Approach

band-gap corrected DFT



Predicted electronic levels in ZnO

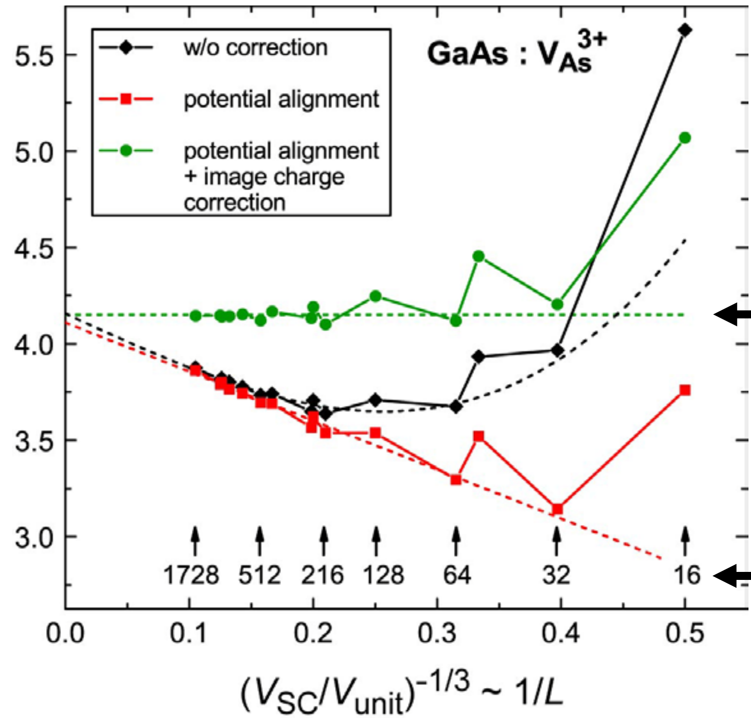


[1] "Electronic structure, donor/acceptor transitions, and magnetism of 3*d* impurities in In_2O_3 and ZnO" *H. Raebiger, S. Lany, A. Zunger,* submitted (2009).

[2] "Magnetic interactions of Cr-Cr and Co-Co impurity pairs in ZnO within a band-gap corrected density-functional approach", *S. Lany, H Raebiger, A. Zunger,* Phys. Rev. B **77**, 241201(R) (2008).

Scientific/Technical Approach

- **Theory of dopants and defects in PV materials is based on supercell methods: How well are finite-size effects under control? (Literature is controversial)**
- **We demonstrated robust and accurate method to determine supercell energies**



Approach:
Test method by explicit calculation of large supercells

size-dependence eliminated after appropriate treatment of supercell effects

supercell size

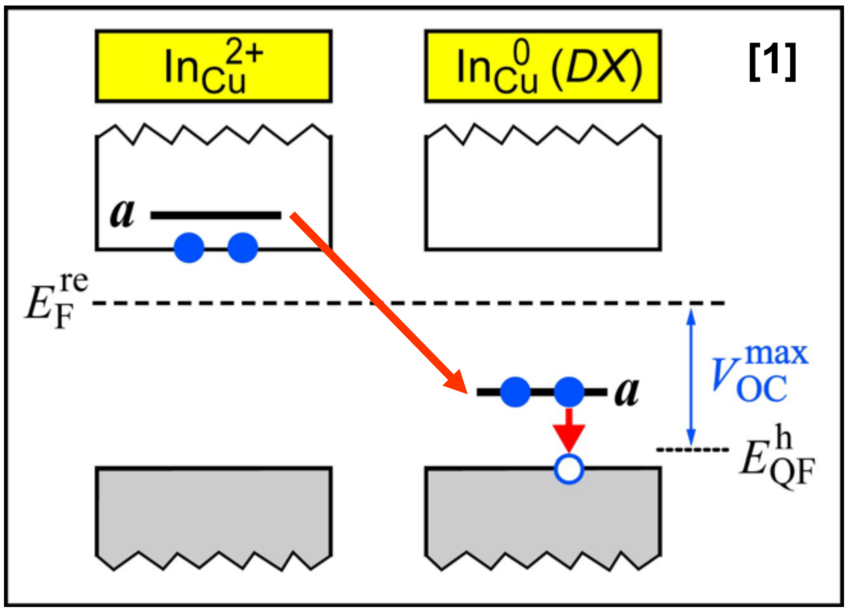
Significance:
Quality-check of theory predictions

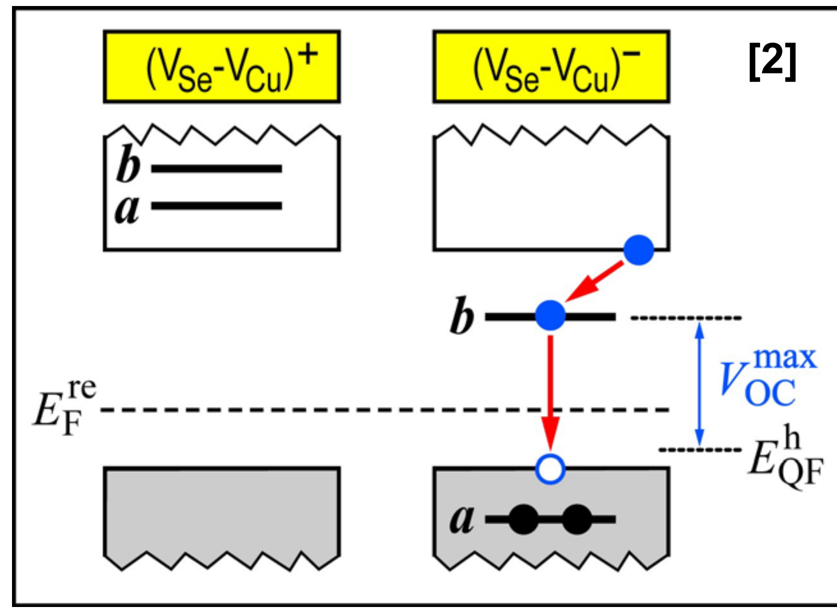
[1] "Assessment of correction methods for the band gap problem and for finite-size effects in supercell defect calculations: Case studies for ZnO and GaAs" *S. Lany, A. Zunger,* Phys. Rev. B **78**, 235104 (2008).

Scientific/Technical Approach

Theory of Transparent Conductors

- **Open-circuit voltage does not increase in proportion to the absorber band gap**
  What causes the performance limitation in $Cu(In,Ga)Se_2$ technology?
- **We identified two types of defects that act to annihilate electron-hole pairs**





[1] "Intrinsic *DX* centers in ternary chalcopyrite semiconductors" *S. Lany, A. Zunger,* Phys. Rev. Lett. **100**, 016401 (2008).

[2] "Light- and bias-induced metastabilities in $Cu(In,Ga)Se_2$ based solar cells caused by the $(V_{Se}\text{-}V_{Cu})$ vacancy complex", *S. Lany, A. Zunger,* J. Appl. Phys. **100**, 113725 (2006).

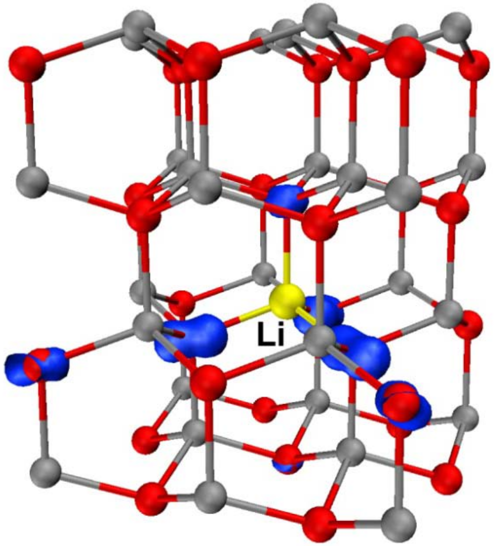
Scientific/Technical Approach

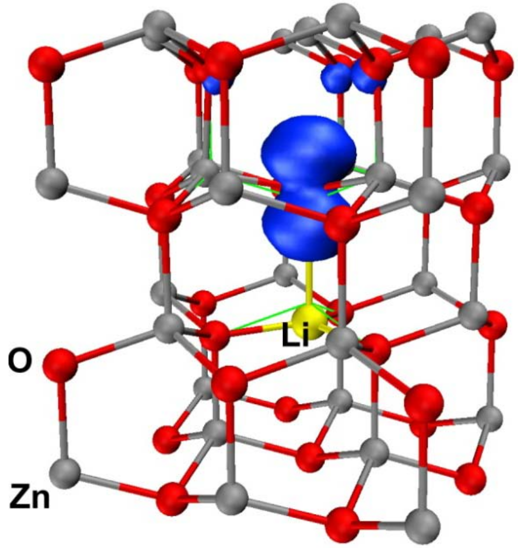
Theory of Transparent Conductors

- **Goal:** **Predict *p*-type TCO**
- **Problem:** **Standard density functional theory (DFT) predicts wrong hole-state**
- **Solution:** **Define hole-state potential V_{HS} to remove DFT bias for delocalization**

Example: Li acceptor in ZnO

Standard DFT (wrong) ***DFT + V_{HS} (correct)***





Results: Acceptor levels in ZnO, In_2O_3 and SnO_2

ZnO:	**Li**	**Na**	**Cu**	**Ag**
E_A (eV)	0.9	0.8	2.3	1.2
In_2O_3:	**Be**	**Mg**	**Ca**	**Zn**
E_A (eV)	1.3	0.9	0.7	1.0
SnO_2:	**B**	**Al**	**Ga**	**In**
E_A (eV)	1.6	0.9	0.8	0.6

[1] "Prediction of polaronic hole states in oxides without bias"
S. Lany, A. Zunger, in preparation (2009).

Relevance/Impact of Research

- Built cutting-edge capabilities to predict PV materials: Absorbers, *n*-type TCO, *p*-type TCO
- Predicted behavior of transition metal impurities in *n*-type TCO: ZnO, In_2O_3
- Identified bottlenecks in current $Cu(In,Ga)Se_2$ technologies

Future Directions

- **PV materials by design: Use unique capabilities to predict and design new PV materials (In-free absorbers; new TCO's; new absorbers); ready to embark on large, interdisciplinary project that is poised to make significant advances in critical PV materials.**

Quality, Productivity, Accomplishment

PV MaterialsTheory

- Task is led by Suhuai Wei and Computational Material Science Team, which has strong experience in developing theory of PV materials and performing state-of-the-art theoretical modeling and calculations. The team has an excellent publication record in the field of PV materials study. Suhuai Wei has been invited speaker at many international conferences on energy related materials.

- The team utilizes NREL's HPC clusters and the DOE supercomputer facility at NERSC

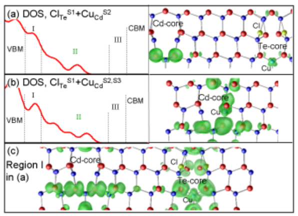
- Strong interaction with NREL's experimental work with several joint publications with experimental groups

- Due to limited PV funding, postdocs hired under other DOE programs have charged to this PV task and made significant contributions toward project milestones.

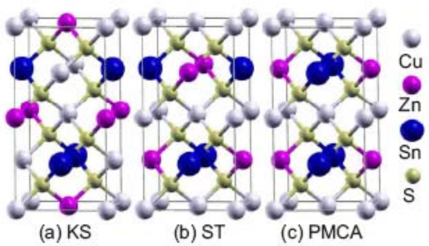
Budget:

- \$340K in FY08; \$390K in FY09 (CR)

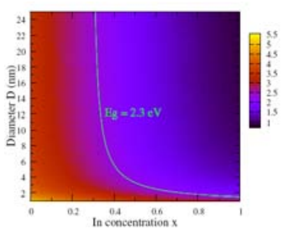
FY09 Publications (up to February, 2009):



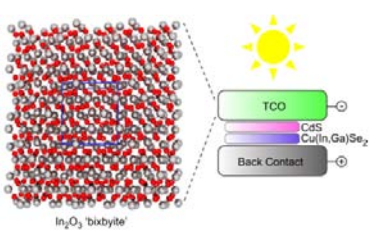
- Studied the structural and electronic properties of grain boundaries (GB) in polycrystalline CdTe--**Significance**: Explained the importance of co-passivation of Cl and Cu on CdTe GB in improving the efficiency of CdTe-based solar cell [L. Zhang et al., Phys. Rev. Lett. **101**, 155501 (2008).]



- Investigated crystal and electronic band structure of Cu_2ZnSnX_4 (X=S, and Se)--**Significance**: Identified several potential low-cost and high efficient photovoltaic absorbers [Chen et al., Appl. Phys. Lett. **94**, 041903 (2009).]



- Demonstrated superb strain relaxation and band-gap tunability in ternary $In_xGa_{1-x}N$ nanowires--**Significance**: Suggested of using $In_xGa_{1-x}N$ nanowires for potential high-efficiency multijunction solar-cell applications [H. J. Xiang et al., Phys. Rev. B **78**, 193301 (2008).]



- Our work on symmetry-induced transparency in conductive metal oxides is highlighted by SPIE Newsroom--**Significance**: Provided guideline for searching efficient TCO for optoelectronic (Solar cell) applications [A. Walsh et al., **DOI**: 10.1117/2.1200810.1368; Phys. Rev. B (in press).]

(Eight additional publications in FY08, see project summary)

Scientific/Technical Approach

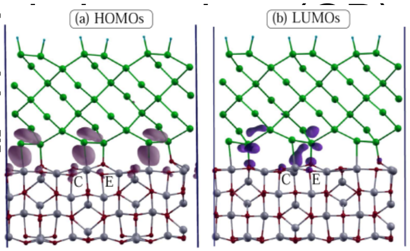
- Use state-of-the-art computational tools to establish the fundamental knowledge infrastructure of PV materials. Our study is two-fold: (i) explain experimental results and providing guidance for future experimental investigation, and (ii) propose design of new PV materials which are potential candidates for future PV applications.

- Work in close collaboration with NREL experimental groups. Our calculated results are shared with them for test and confirmation. Experimental results are in turn used to guide our future research activities.

Relevance/Impact of Research

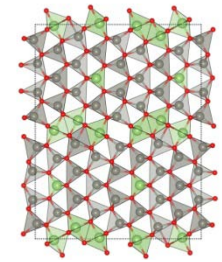
PV MaterialsTheory

- Goal: enhance and accelerate the advances in the national photovoltaic technology and R&D program defined in the road maps. Improve solar cell efficiency and reduce its cost through understanding and control of material properties. Examples of recent study include:
  - Solar cells made of thin c-Si film (10-20 μm) grown on inexpensive metal oxide substrates have great potential to significantly reduce the cost, while maintaining the efficiency of wafer-based Si solar cells. To achieve optimal performance, understanding the microscopic structure of the interface is very important.
  - InZnO, GaZnO, and AlZnO are currently considered as good candidates of TCO to replace the high cost ITO used in optoelectronic devices such as solar cells. Understanding their structural, electronic and optical properties is crucial for their applications.
  - Understanding passivation mechanism at the gr
    and defect diffusion in bulk and GB region is imp
    the efficiency of CdTe- and CIGS-based solar c



Future Directions

PV MaterialsTheory



- Unravel the microscopic structure of the c-Si/Al_2O_3 interface in order to achieve better solar cell performance; search the best oxide substrate for thin-film c-Si growth

- Understand microscopic structure and passivation mechanism of the c-Si/a-Si heterojunction interfaces in order to improve the cell efficiency

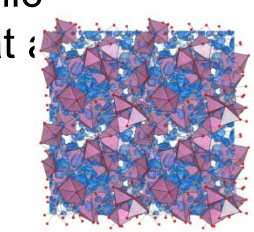
- Study the atomic structure and passivation of dislocations at lattice mismatched semiconductor interfaces, which are key to the success of iLMM and GaInN based solar cell.

- Understand the role of Cu and Cl diffusion in CdTe-based solar cell system, calculate the diffusion barriers of Cu and Cl in CdTe, CdS, ZnTe, $CdTeO_3$, CuO

- Study the electronic, structural, and defect properties of CdMTe (M=Mg, Zn) alloys, which could be used to improve the V_{oc} or for high efficiency CdTe-based tandem solar cells

- Obtain the electronic and optical properties of the crystalline and amorphous phases of the homologous $InMO_3(ZnO)_n$ (M=Al, Ga, In) alloys for possible TCO application

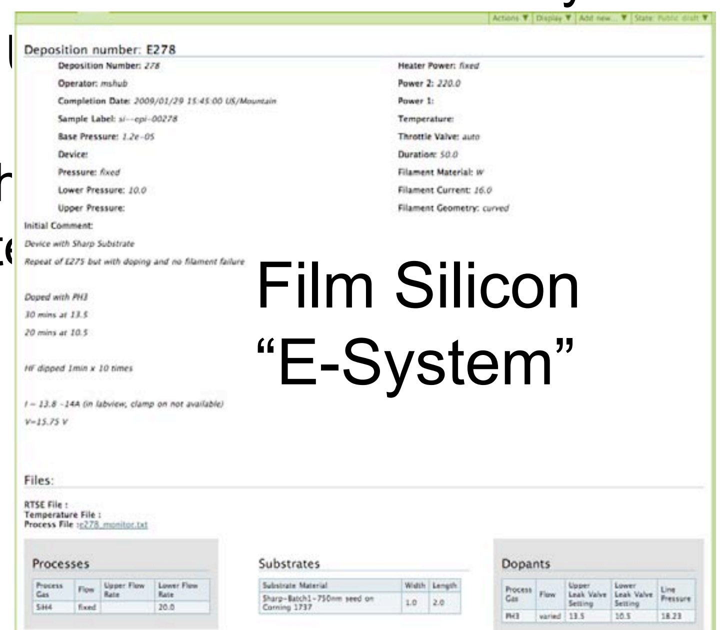
- Modifying the band structure of zinc-blende and chalcopyrite materials through atomic mutation, (e.g, ZnS -> $CuGaS_2$ -> Cu_2ZnGeS_4), identify the quaternary compounds that a suitable for PV applications.



Quality, Productivity, Accomplishment

Scientific Data Mgmt/Mining

- New task in FY09 - Our team is composed of a mix of PhD researchers, computing specialists, and programmers with scientific backgrounds. We have a track record of developing useful data tools in collaboration with scientists.
- A recent hire specializing in materials informatics is uniquely qualified to lead this effort and provides a unique opportunity for the Solar Program to leverage this emerging set of techniques and technologies for process improvement and scientific discovery.
- Current funds cover about ½ person. U of contracts, collaborations with universities and postdoctoral research has enabled accomplishments to date



Film Silicon "E-System"

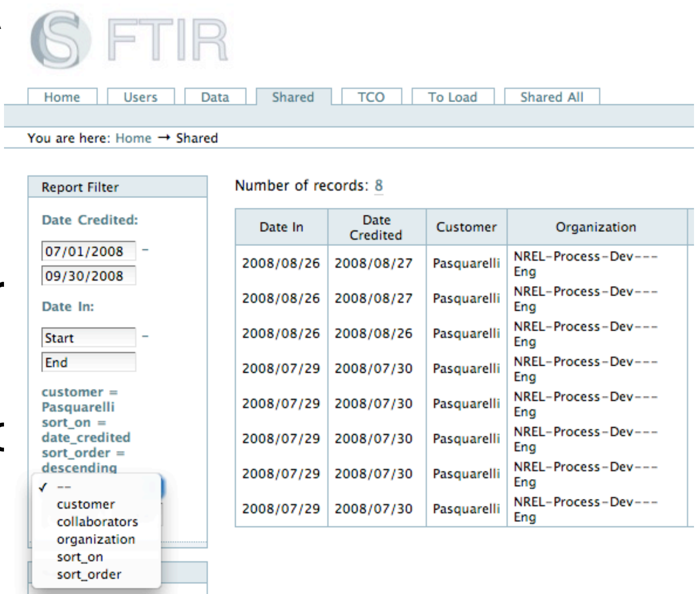
Budget:

- $200K in FY09 (CR)

Quality, Productivity, Accomplishment

Scientific Data Mgmt/Mining

- Initiated and continued work in data aggregation, analysis, and mining
- Master degree awarded to Daniel Korytina for data tools developed in support of the Solar Technologies Program
- Hired Changwon Suh: material informatics postdoctoral researcher; poster on Material Informatics accepted to MRS Spring Meeting, '09
- Updated data aggregation tool for silicon deposition "E-System" focused on data entry and record displa
- Updated data aggregation tool for FTIR focused on data access and reporting
- Created new repository for TCO "cube" deposition system; expressed repositor for "data mining"
- Initiated collaboration with OPV group fc data aggregation
- Participated in NREL "Informatics



Scientific/Technical Approach

Scientific Data Mgmt/Mining

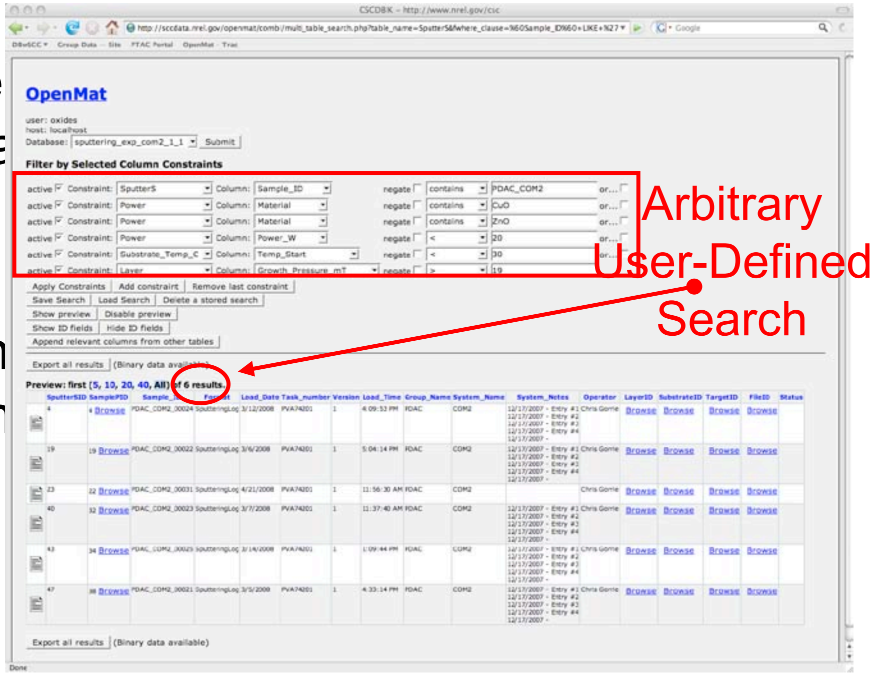
- Build small sustainable working systems focused on data models and access within open source enterprise framework. Build sophisticated data management and aggregation tools to relate deposition, characterization, and process data and enable “mining” of related data. Use agile techniques to enable incremental improvement in researchers ability to aggregate, access and search data.
- Understand, develop and apply state of the art material informatics techniques, design of experiments and optimization techniques in collaboration with research scientists.
- Collaborate with researchers on needs and develop infrastructure, techniques and methodologies that may be applied by researchers investigating different solar technologies.
- MRS Bulletin, 2006, “The constant quest for new materials, improved performance, decreased development costs, and reduced environmental impact ensure the steadily growing importance of systematic materials development….. These computational approaches, collectively termed “materials informatics,” provide an effective way to interpret and use material properties data in the selection and design of materials products.”

Task	WSi	FSi	CPV	CdTe	CIGS	OPV	TCO	PDIL	EOC
1 Scientific Data Management		X		X		X	X	X	X

Relevance/Impact of Research

Scientific Data Mgmt/Mining

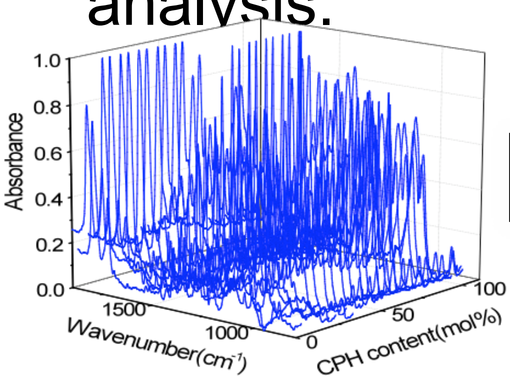
- The focus of this task is to enable the understanding and discovery of processes and materials for solar applications and in support of solar technologies through systematic and intelligent application of aggregation, analysis and mining (informatics) techniques to scientific and technical data.
- The development and application of expertise, capabilities and infrastructure is focused on accelerating the design, discove and improvement of processes a materials.
- The approach is grounded in developing core capabilities with application through collaboration with solar technology program researchers.



Future Directions

Scientific Data Mgmt/Mining

- Establish data management, analysis, mining and informatics as a core, valued asset in support of the Solar Program goal
- Establish core knowledge, expertise (staffing) and capabilities in support of this asset as its value is recognized and increases
- Hire a statistician to enable use of design of experiments, advanced dimension reduction, multivariate analysis, regression, and signal to noise analysis.



Dimension reduction enables understanding of relationships