EXPLORE AND COLLABORATE
AMERICAN INDUSTRY AND AMERICA'S NATIONAL LABS
MATERIALS FOR ENERGY APPLICATIONS

HIGH-PERFORMANCE COMPUTING CAPABILITIES WITHIN DOE

Leveraging computing to accelerate materials development and deployment

High-performance computing (HPC) **accelerates the development and deployment of materials** for renewable energy technologies by *(i)* providing fundamental insight into materials performance and characteristics, *(ii)* complementing and aiding the interpretation of advanced characterization, and *(iii)* creating a virtual laboratory to explore composition and processing options. DOE's HPC resources enable ***predictive first-principles simulations*** at technologically-relevant length and time scales, as well as ***high-complexity multi-scale simulations***, driving the state-of-the-art.

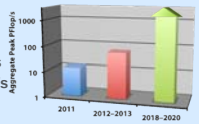
Leadership-Class Supercomputing

Today and Into the Future

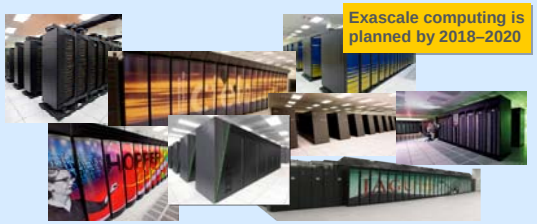
DOE Labs house 20 of the TOP 100 supercomputers in the world and 21% of peak computing power in the TOP 100 (13.4 PetaFlop/s on 1.64M computing cores, in aggregate)

By 2012–2013, 60+ PFlop/s will be achieved with 3 new leadership supercomputers:

- **LLNL's Sequoia: 20 PFlop/s**
- **ORNL's Titan: 10–20 PFlop/s**
- **ANL's Mira: 10 PFlop/s**



Exascale computing is planned by 2018–2020



State-of-the-art systems employ advanced architecture technologies, including GPU computing and flash memory storage

Labs as Hub for Industrial Partnerships in HPC

High Performance Computing Innovation Center (HPCIC) within LVOC at LLNL

- Boost American competitiveness by providing industry access to multi-PF HPC resources and expertise
- Partner with industry to provide lower cost and time to solution

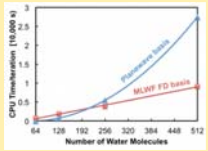
Innovation Center for Computational Research on Energy Advanced Materials (ICeCREAM) at LLNL

- Center in-development to focus efforts in materials modeling for renewable energy technologies, leveraging HPC resources and expertise
- Engage industry and academia

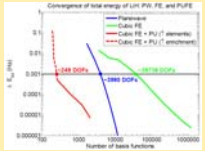
Scalable Methods for Large-Scale First-Principles Materials Simulations

Matching length & time scales of simulations to relevant experimental & technological conditions

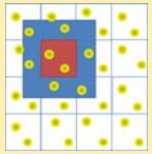
Advanced scalable algorithms enable highly accurate first-principles molecular dynamics simulations with 10,000's+ atoms utilizing 100,000's+ cores



Wannier function localization in real-space enables linear-scaling O(N) solution of DFT for systems with 1000's+ atoms
[J.-L. Fattebert and F. Gygi, *PRB* **73**, 115124 (2006)]



Partition-of-unity finite-element (PUFE) method: same accuracy as traditional methods with order-of-magnitude smaller basis set
[Pask, Sterne, *Mod. Simul. Mater. Sci. Eng.* **13**, R71 (2005); Sukumar, Pask, *Int. J. Numer. Meth. Engng.* **77**, 1121 (2009)]



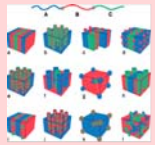
Adaptive local basis method: 1 meV accuracy DFT with only few basis functions per atom, computed on-the-fly and trivially parallelizable
[L. Lin, *et al., J. Comput. Phys.* 231, 2140, 2012]

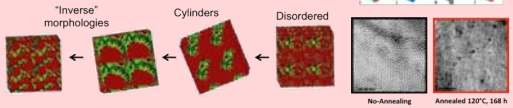
Example Applications

Multiblock Copolymers for Energy Applications

Designer multiblock copolymers may enable high-performance, inexpensive PV & batteries

- Simulations guide design of copolymer synthesis to control morphology & stability
- Multi-length/time scale polymer simulation codes at ORNL being scaled to 10^5–10^6 cores

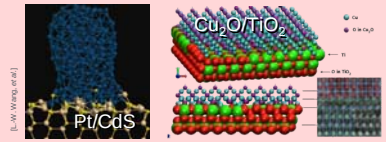




[M. Goswami, B.G. Sumpter, *et al., Soft Matter* **6**, 6146 (2010); X. Wang, B.G. Sumpter, *et al., Soft Matter Commun.* **7**, 7960 (2011)]

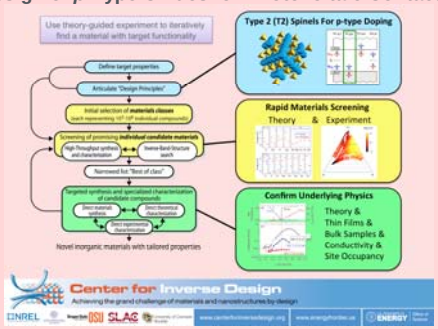
Realistic Interface Modeling

Large supercomputers enables realistic modeling of material interfaces — relevant for PV, photo/electro-catalysts, etc.



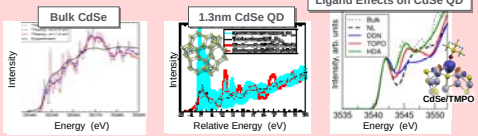
1000's of atoms required for realistic interfaces

Design of *p*-Type Oxides for Photovoltaic Contacts



X-Ray Spectroscopy Simulations

Predictive X-ray spectra simulations coupled with experiments at advanced light-source facilities provides a powerful tool to correlate the atomic structure of new materials with properties

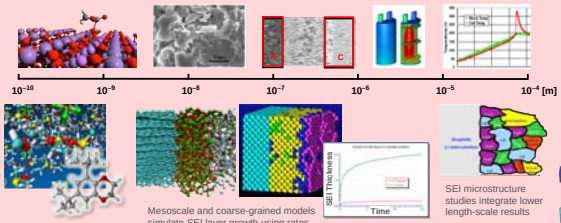


Example: Ligand-tuning of optical properties of CdSe QDs for PV

[D. Prendergast & G. Galli, *Phys. Rev. Lett.* (2006); J.S. Uejio, *et al., Chem. Phys. Lett.* (2008); H. Whitley, *et al.*, (2010)]

Multiscale, Multiphysics Modeling of Batteries from Atoms to Cells

[L. Curtis, *et al.* (ANL); R. Muller, *et al.* (SNL); W. Miller, *et al.* (LLNL)]



First-principles models reveal chemistry and mechanisms of electrolyte decomposition at the atomic scale

Mesoscale and coarse-grained models simulate SEI layer growth using rates and mechanisms from first-principles

SEI microstructure studies integrate lower length-scale results

High fidelity multi-physics simulations probe catastrophic failure and provide virtual testing platform

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