Session S19: Building the Bridge to Exascale: Applications and Opportunities for Materials, Chemistry, and Biology I

Show Abstracts

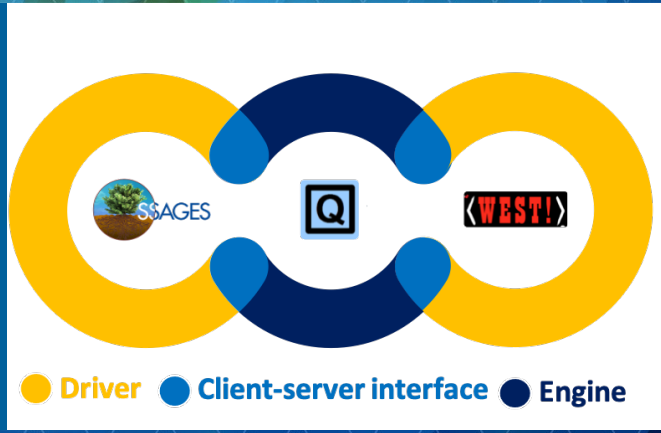
Focus Live

Sponsoring Units: DCOMP DCMP DAMOP DCP
Chair: Jack Deslippe, Lawrence Berkeley National Laboratory

Thursday, March 18, 2021 11:30AM - 12:06PM Live	S19.00001: Accelerating Large-Scale Excited-State GW Calculations on Leadership Class HPC Systems Invited Speaker: Mauro Del Ben
Thursday, March 18, 2021 12:06PM - 12:18PM Live	S19.00002: From LSMS to MuST: Large scale first principles materials calculations at the exascale Markus Eisenbach, Xianglin Liu, Mariia Karabin, Swarnava ghosh, Yang Wang, Hanna Terletska, Wasim Mondal, Ka-Ming Tam, Yi Zhang, Liviu Chioncel
Thursday, March 18, 2021 12:18PM - 12:30PM Live	S19.00003: Recently Added Features, Scaling and Performance of the Real-Space MultiGrid (RMG) Code on Exascale Architectures Emil Briggs, Wenchang Lu, Jerry Bernholc
Thursday, March 18, 2021 12:30PM - 12:42PM Live	S19.00004: QMCPACK's Exascale Performance Portability Strategies Paul Kent, Peter Doak, Mark Dewing, Ye Luo
Thursday, March 18, 2021 12:42PM - 12:54PM Live	S19.00005: A Pseudo-BCS Wavefunction from Density Matrix Decomposition: Application in Auxiliary-Field Quantum Monte Carlo Zhi-Yu Xiao, Hao Shi, Shiwei Zhang
Thursday, March 18, 2021 12:54PM - 1:06PM Live	S19.00006: GPU-Acceleration of the ELPA2 Distributed Eigensolver for Applications in Electronic Structure Theory Victor Yu, Jonathan Moussa, Pavel Kus, Andreas Marek, Peter Messmer, Mina Yoon, Hermann Lederer, Volker Blum
Thursday, March 18, 2021 1:06PM - 1:18PM Live	S19.00007: Discrete discontinuous basis projection (DDBP) method for large-scale electronic structure calculations. Qimen Xu, Phanish Suryanarayana, John Pask
Thursday, March 18, 2021 1:18PM - 1:30PM Live	S19.00008: MERA++: An Implementation of the Multi-scale Entanglement Renormalization Ansatz Gonzalo Alvarez
Thursday, March 18, 2021 1:30PM - 1:42PM Live	S19.00009: Matrix Product States in the Continuum and Cold Atomic Gases Clayton Peacock, Aleksandar Ljepoja, Carlos J Bolech
Thursday, March 18, 2021 1:42PM - 1:54PM Live	S19.00010: Overcoming the noncausality problem in nonlocal extensions of dynamical mean-field theory Steffen Backes, Jae-Hoon Sim, Silke Biermann
Thursday, March 18, 2021 1:54PM - 2:06PM	S19.00011: Coupling interoperable software for quantum simulations of materials Marco Govoni, He Ma, Nan Sheng, Sijia Dong, Francois Gygi, Giulia Galli
Thursday, March 18, 2021 2:06PM - 2:18PM	S19.00012: Implementation of spin-orbit coupling in the Real-space MultiGrid (RMG) code Wenchang Lu, Emil Briggs, Jerry Bernholc, Anh Pham, Panchapakesan Ganesh
Thursday, March 18, 2021 2:18PM - 2:30PM	S19.00013: Magnetic and charge orders in the ground state of the 2D repulsive Hubbard model Hao Xu, Mingpu Qin, Hao Shi, Yuan-Yao He, Ettore Vitali, Shiwei Zhang

APS March Meeting 2021
Building the Bridge to Exascale: Applications and Opportunities for Materials, Chemistry, and Biology I – March 18th, 2021

COUPLING INTEROPERABLE SOFTWARE FOR QUANTUM SIMULATIONS OF MATERIALS

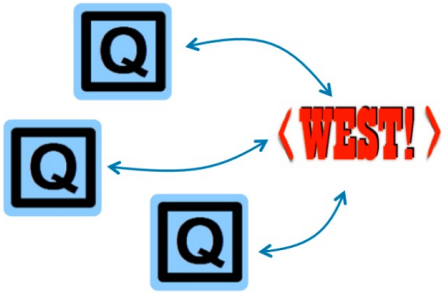


MARCO GOVONI[1,2], HE MA[2], NAN SHENG[2], SIJIA DONG[1], FRANCOIS GYGI[3], GIULIA GALLI[1,2]
[1]Argonne National Laboratory
[2]University of Chicago
[3]University of California Davis

OUTLINE

- **New simulation techniques leverage interoperable software**

The Qbox-WEST coupling enables the calculation of:



M. Govoni et al., npj Comput. Mater. 7, 32 (2021)

- Optical absorption spectra harnessing orbital localization

Machine Learning

TensorFlow

Nguyen et al., *PRL* 122, 237402 (2019)
Dong et al., *Chem. Sci.*, Advance Article (2021)

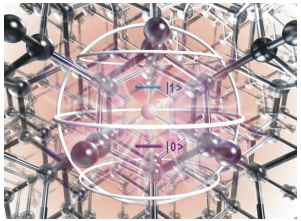
- Highly-correlated electronic states

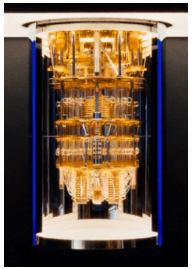
Quantum Computing

Qiskit

Ma et al., npj Comput. Mater. 6, 85 (2020)
Ma et al., *PCCP* 22, 25522 (2021)
Ma et al., *JCTC* accepted (2021)

Results for spin-defects, applications in quantum information science



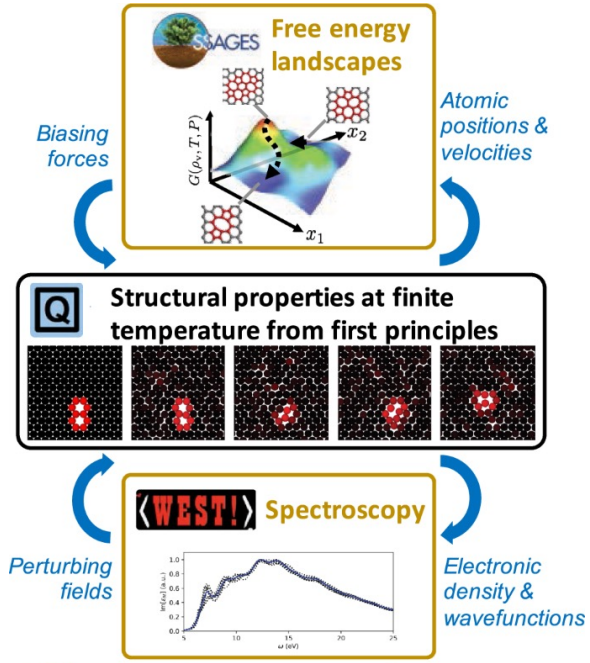


COUPLING INTEROPERABLE SOFTWARE

Emerging trend in computational materials science: development of codes that singly carry out specific tasks…

- **SSAGES**: advanced sampling
- **Qbox**: first-principles molecular dynamics
- **WEST**: many-body perturbation theory

…and cooperatively perform complex simulations



SSAGES-Qbox
Advanced sampling using first principles molecular dynamics simulations

WEST-Qbox
Spectroscopy from first principles
- Optical absorption
- Highly-correlated electronic states

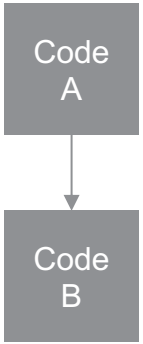
https://ssagesproject.github.io
http://qboxcode.org
http://west-code.org

M. Govoni et al., npj Comput. Mater. 7, 32 (2021)

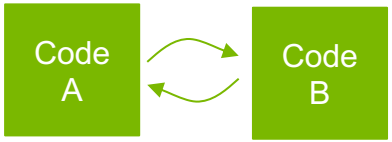
MODULAR COMPUTATIONAL STRATEGY

- Challenges of interfacing codes:
  - **lack of standardized procedures** for sharing information between the codes (different data structures, file formats, units and coding language)
  - Codes may require to **run concurrently** and communicate frequently
- A modular strategy is critical for:
  - **Maintainability**, **re-usability**, **extensibility**
  - Ensuring backward compatibility of syntax for the coupling is the only requirement to maintain code interoperability, and the remaining details of the implementation of each code are not restricted

ex vivo coupling

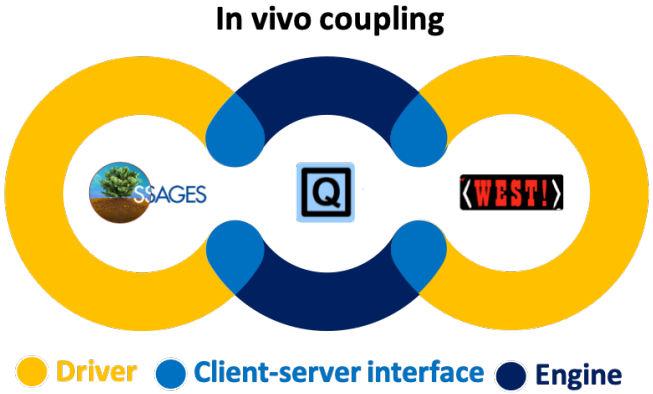


in vivo coupling



CLIENT-SERVER INTERFACE

- Within the **client-server** model:
  - Multiple servers may be used to distribute computationally intensive workloads
  - Synchronization operations occur through interaction via the file system (negligible overhead)
  - A markup language (XML) is used to document exchanged datasets
  - The execution of multiple runs of similar sets of tasks is facilitated by keeping information in memory between sessions



M. Govoni et al., npj Comput. Mater. 7, 32 (2021)

The **driver** program acts as a client and sends a set of instructions to an **engine** code acting as a server

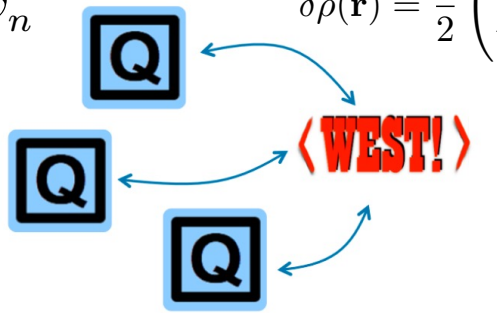
WEST-QBOX COUPLING

- The WEST-Qbox coupling enables the direct calculation of the dielectric screening, without the evaluation of a dielectric matrix
- The linear variation of the charge density *induced* by a perturbative potential is

$$\left(H_{KS} \pm \delta V_{pert}\right) \psi_n^{\pm} = \varepsilon_n \psi_n^{\pm}$$

$$\delta\rho(\mathbf{r}) = \frac{1}{2}\left(\sum_n^{occ} \left|\psi^+(\mathbf{r})\right|^2 - \left|\psi^-(\mathbf{r})\right|^2\right)$$

each **Qbox** instance computes the electronic response to given perturbations (client/server mode)



Exchanged one 3D field

WEST outsources the calculation of the electronic response

http://qboxcode.org/
Gygi, *IBM J. Res. Dev.* 52 p.137 (2008)

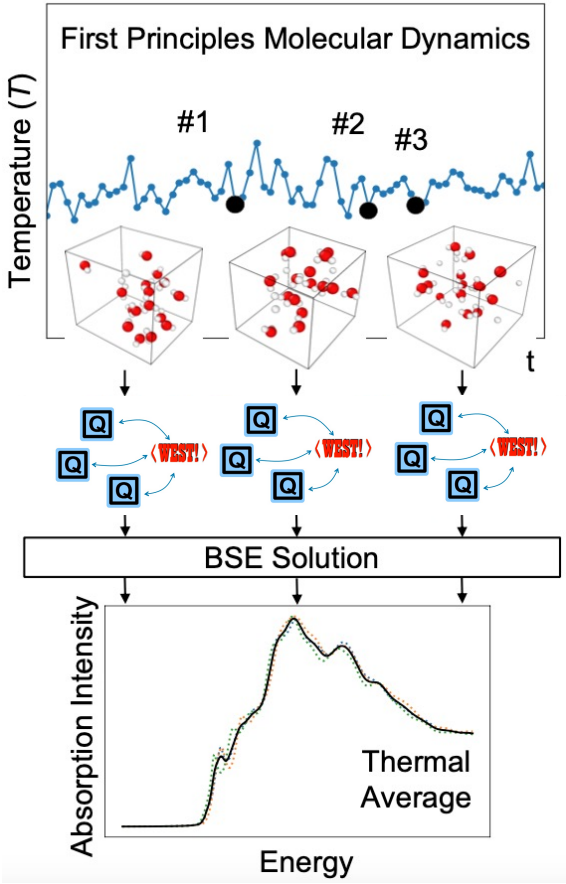
http://west-code.org
Govoni et al., *JCTC* 11, 2680 (2015)
Ma et al., *JCTC* 15, 154 (2019)
M. Govoni et al., npj Comput. Mater. 7, 32 (2021)

FINITE T OPTICAL ABSORPTION

Optical absorption is simulated from first-principles by solving the Bethe-Salpeter equation

Challenge: calculation of dielectric matrix for several snapshots extracted from MD trajectory

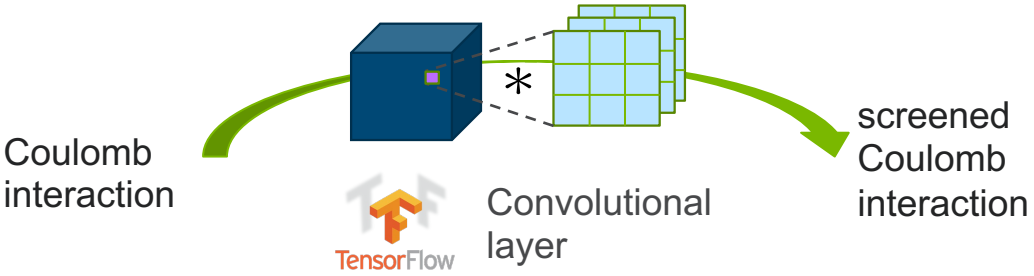
- Defined a finite field approach to solve BSE within the Liouville-Lanczos method:
  - Used **WEST-Qbox coupling** to avoid direct calculation of dielectric matrices and overcome a few commonly used approximations (e.g., RPA)
  - Obtained **reduced scaling** by harnessing orbital localization (recursive bisection method)

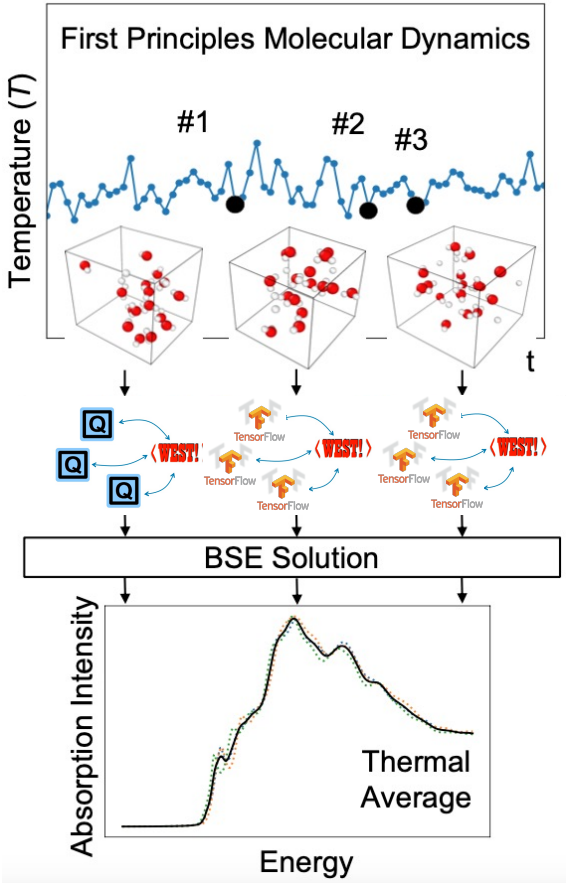


Nguyen et al., *PRL* 122, 237402 (2019)
Gygi, *PRL* 102, 166406 (2009)

FINITE T OPTICAL ABSORPTION

- Identified a **machine learning** protocol to “learn” the dielectric response on-the-fly
  - Speedup 100x
  - model dielectric functions may be derived





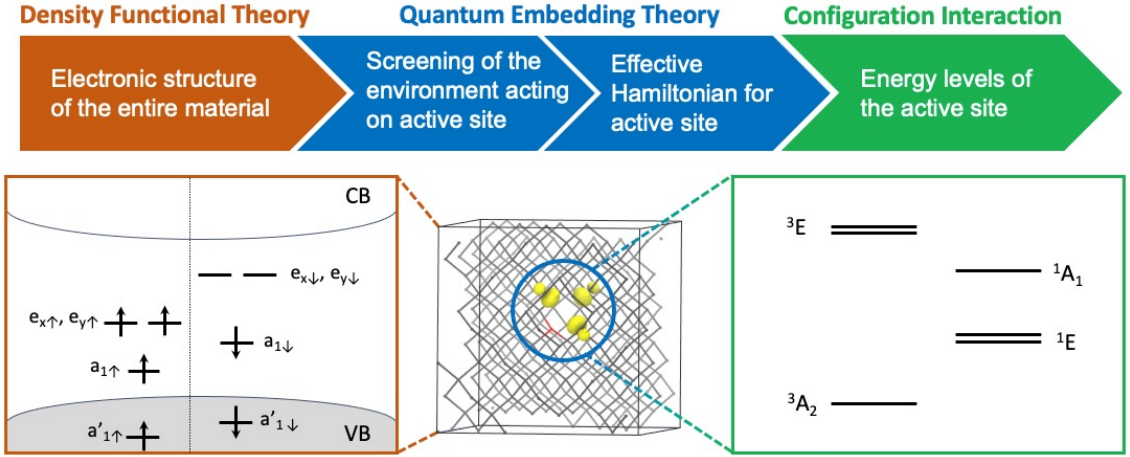
Dong et al., Chem. Sci. Advanced article (2021)

HIGHLY CORRELATED ELECTRONIC STATES

Highly correlated electronic states of **active regions** (e.g., defects) in materials may be computed using a quantum embedding theory

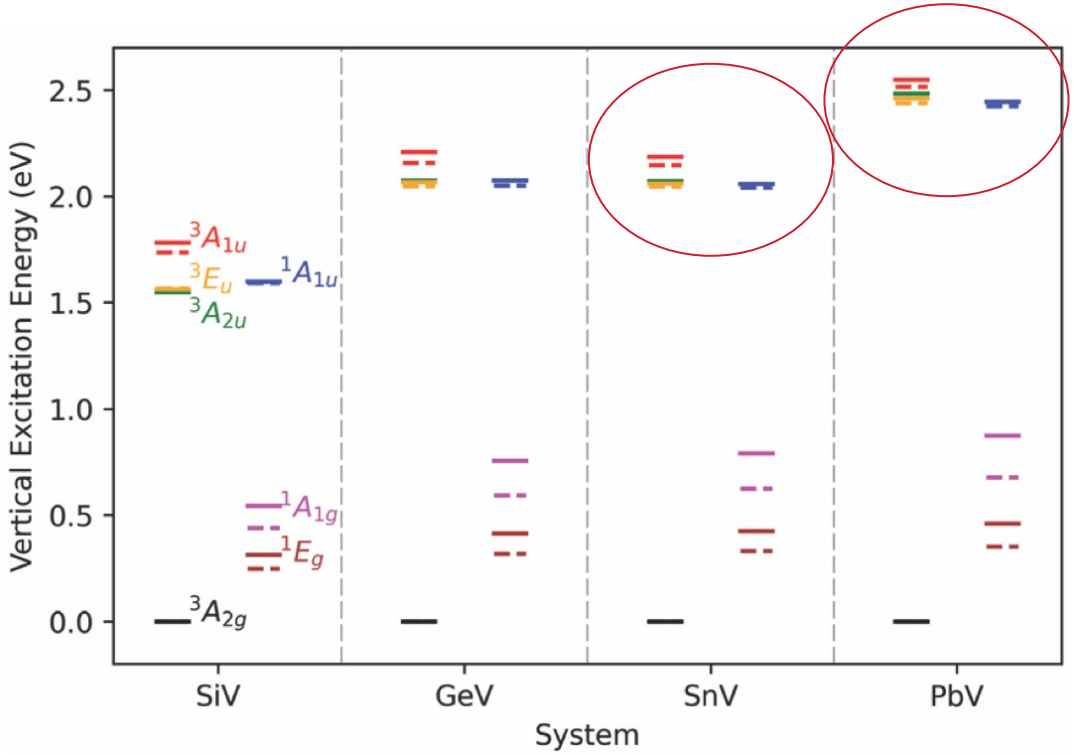
Challenge: within the constrained RPA formalism one has to compute a partial dielectric screening (screened only by the host, described within DFT)

- The WEST-Qbox coupling enables the calculation of the partial dielectric response beyond the RPA and for large systems (no empty states)



SPIN-DEFECTS MODELING

- Demonstrated accuracy of the method by investigating several spin-defects in semiconductors
- For group-IV defects in diamond, we **provide a possible explanation for** the experimental difficulty to perform optical spin polarization of SiV^0, and **predict** a possible intersystem crossing in SnV^0 and PbV^0



Ma et al., npj Comput. Mater. 6, 85 (2020)
Ma et al., *PCCP* 22, 25522 (2021)
Ma et al., *JCTC* accepted (2021)

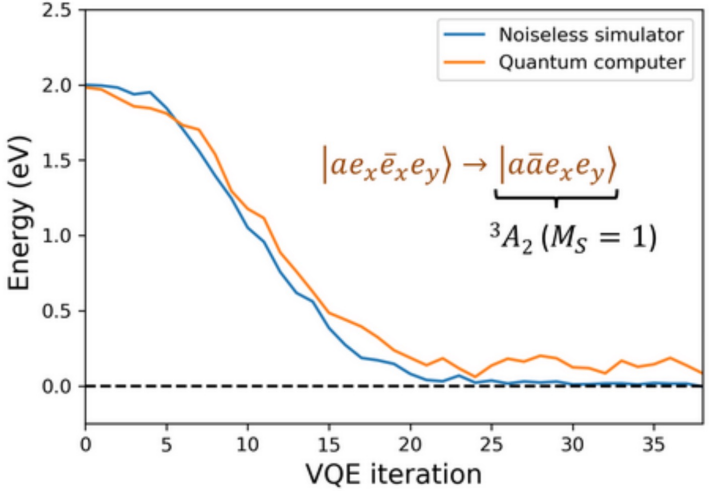
CORRELATED MATERIALS STUDIED WITH QUANTUM COMPUTERS

Demonstrated the use of the variational quantum eigensolver (VQE) to solve on IBM quantum resources the effective Hamiltonian of the active site with parameters obtained from first principles

Qiskit

pyscf

Calculation of the energy of $^3A_2$ state for NV center in diamond (the host material is treated with DFT)



Ma et al., npj Comput. Mater. 6, 85 (2020)

CONCLUSION

- We presented the coupled use of **WEST and Qbox** to advance the first-principles calculation of:
  - Optical absorption at finite temperature
  - Strongly correlated electronic states in materials
- Together the two codes provide a computational framework for **electronic and optical spectroscopic characterization of complex materials**
- We have also demonstrated:
  - The use of **machine learning** to reduce the number of first-principles calculations
  - The use of **near-term quantum computers** to solve second-quantized quantum algorithms, with input from pre-exascale HPC

ACKNOWLEDGMENTS

- Computational facilities used:
  - ALCF-Theta
  - NERSC-Cori
  - OLCF-Summit
  - IBM Quantum Experience
- Allocations:
  - INCITE
  - Argonne Data Science Program
  - NERSC NESAP
  - IBM Quantum Hub

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MICCoM

U.S. DEPARTMENT OF ENERGY

Thank you!