



# WEST: Novel Scalable Software for Materials by Design

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## The poster in a nutshell

Petascale computational resources have provided the opportunity to perform quantum simulations of materials properties of unprecedented size, yielding results that complement experimental observations and may lead to the **discovery of new materials**, designed using the basic principles of quantum mechanics.

We describe the features of **WEST**, an open source massively parallel code developed to compute excited state properties of molecules and materials.

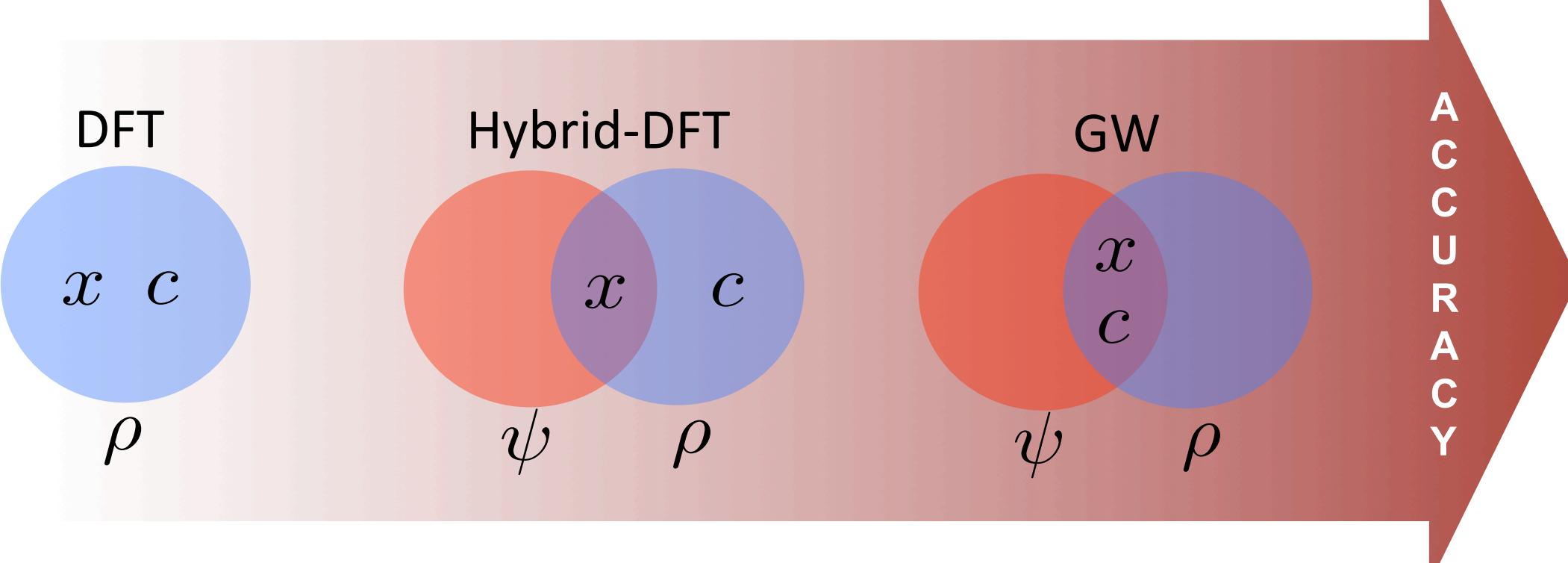


## Motivation

### Materials by design

1. Generate structural models with classical or Ab Initio **Molecular Dynamics**.
2. Carry out **Density Functional Theory** (DFT) electronic structure calculations with semi-local or hybrid functionals.
3. Use DFT input to carry out **Many Body Perturbation Theory** (MBPT) calculations and obtain quasiparticle energies (GW) and absorption properties (BSE).

### Which level of theory?



Understanding materials at the nanoscale and **building predictive capabilities require high accuracy**.

## Large scale GW

In a fashion similar to DFT, **quasiparticle** (QP) states and energies may be obtained replacing the exchange-correlation potential with the **electronic self-energy**  $\Sigma$ .

$$\left( \hat{T} + \hat{V}_{ion} + \hat{V}_H + \hat{\Sigma}(E_n^{QP}) \right) |\psi_n^{QP}\rangle = E_n^{QP} |\psi_n^{QP}\rangle$$

In the GW approximation we have

$$\Sigma(\mathbf{r}, \mathbf{r}'; \omega') = i \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} G(\mathbf{r}, \mathbf{r}'; \omega + \omega') W(\mathbf{r}, \mathbf{r}'; \omega')$$

Challenges: non-locality, retardation effects.

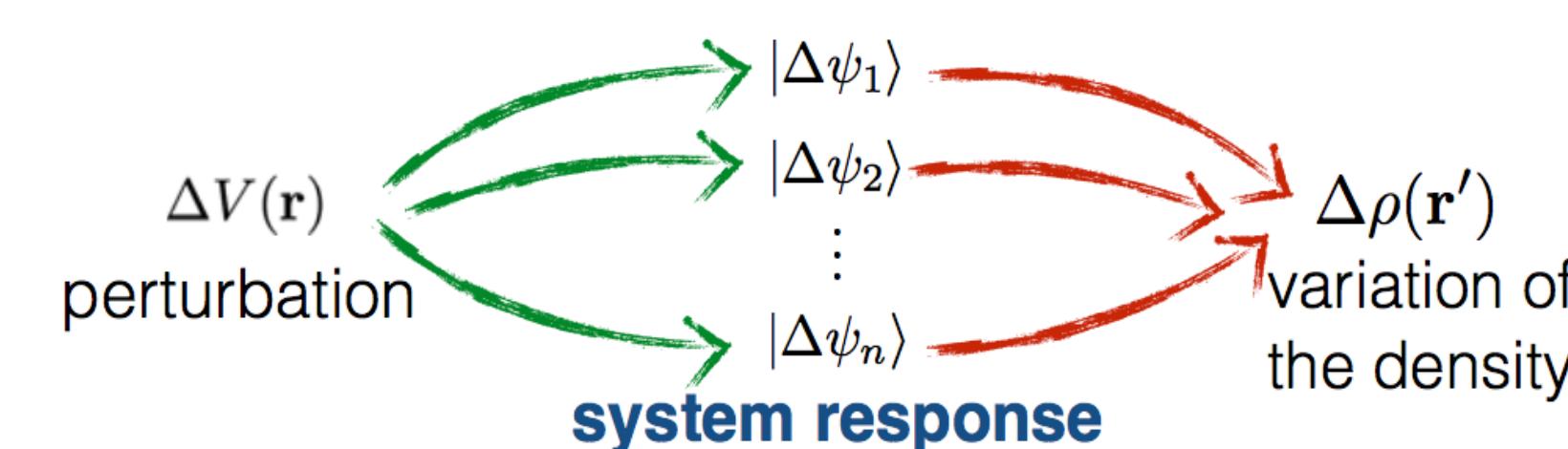
### Algorithmic advances in West

#### #1 The eigen-decomposition of $W$

$$W = \begin{matrix} W \\ \vdots \end{matrix} \times \begin{matrix} \text{eigenpotentials} \\ \vdots \end{matrix} \times \begin{matrix} W \\ \vdots \end{matrix}$$

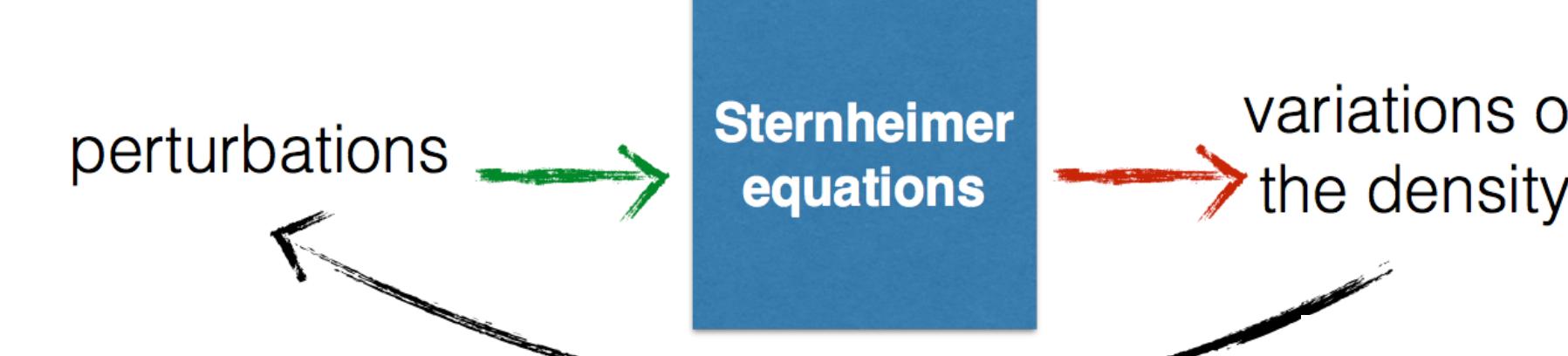
$W = \sum_{\alpha} |\alpha\rangle \lambda_{\alpha} \langle \alpha|$  The number of eigenpotentials controls the accuracy of the method.

#### #2 Linear response with Sternheimer eq.

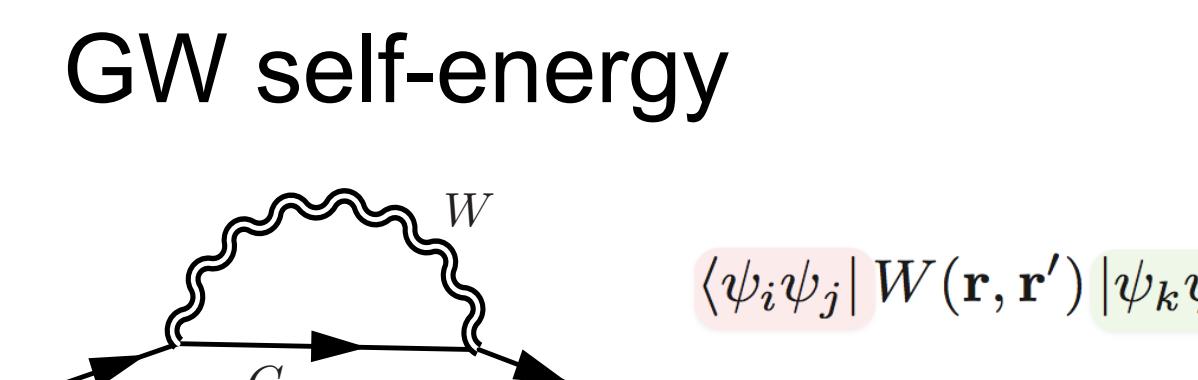
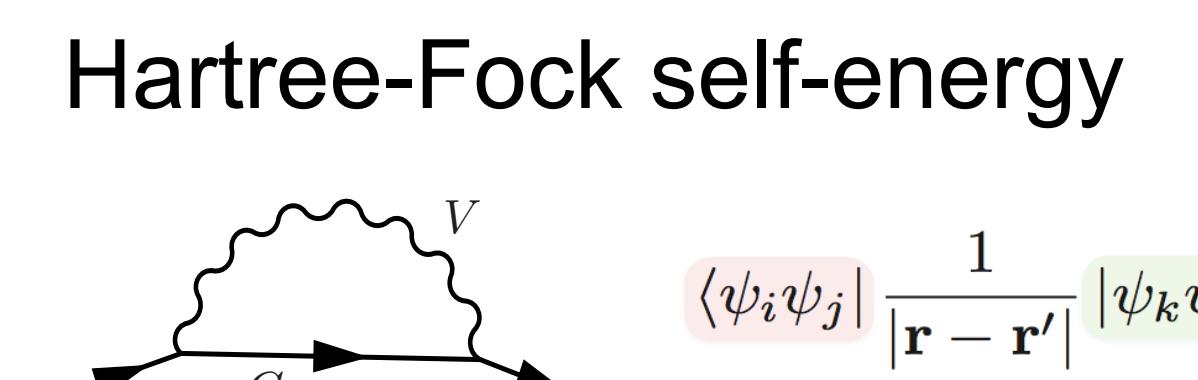


Empty (virtual) states are not involved in the calculation of polarizabilities.

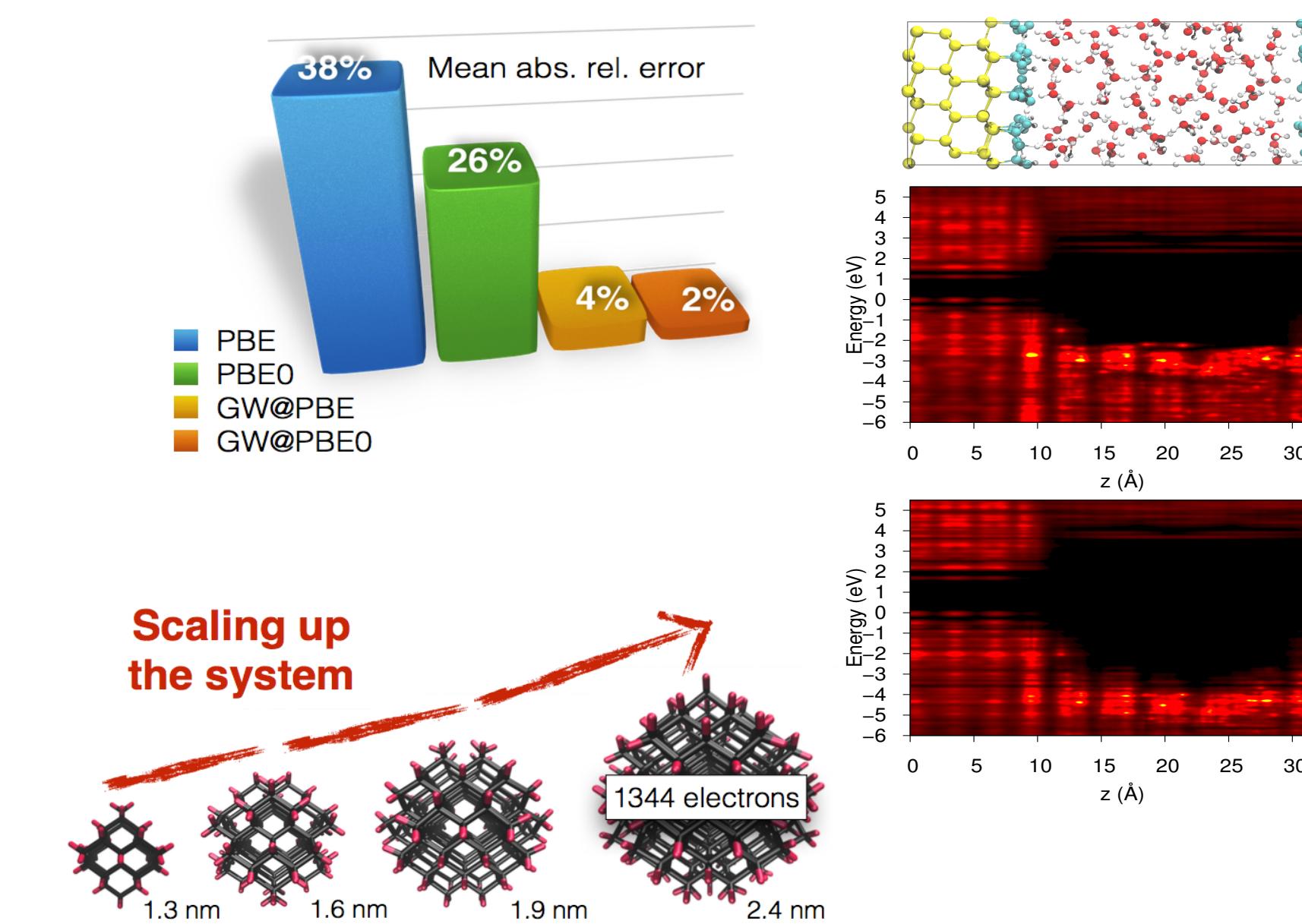
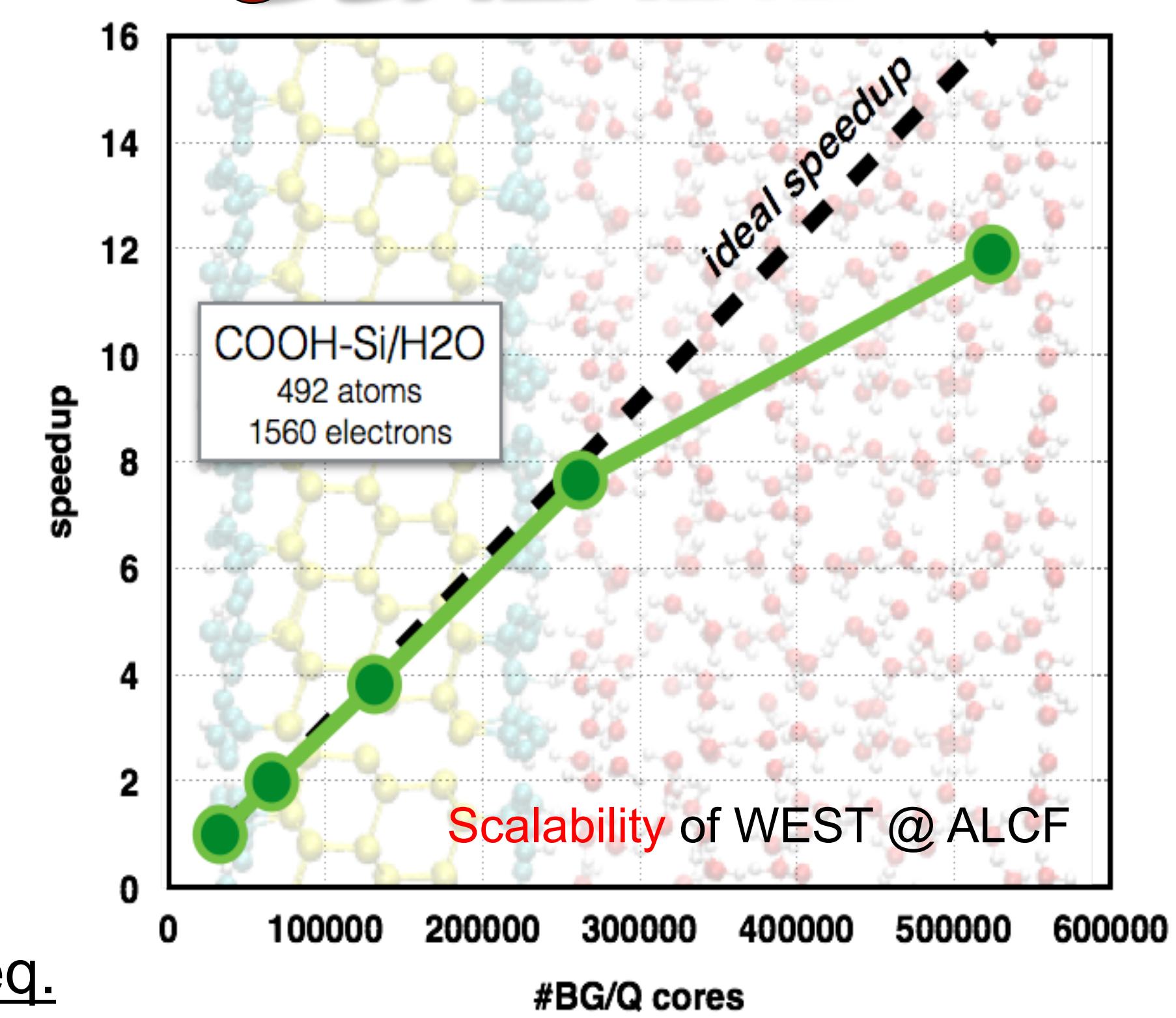
#### #3 Matrix-free diagonalization



Range of applicability: **molecules, solids, liquids, and nanostructures**.



## SCALABILITY



**WEST** can be used for systems with **impurity levels** and to investigate semiconductor surfaces interfaced with aqueous solutions containing ions and to study the influence of ions on the electronic structure of the **interface**.

## Impact

### Energy Conversion

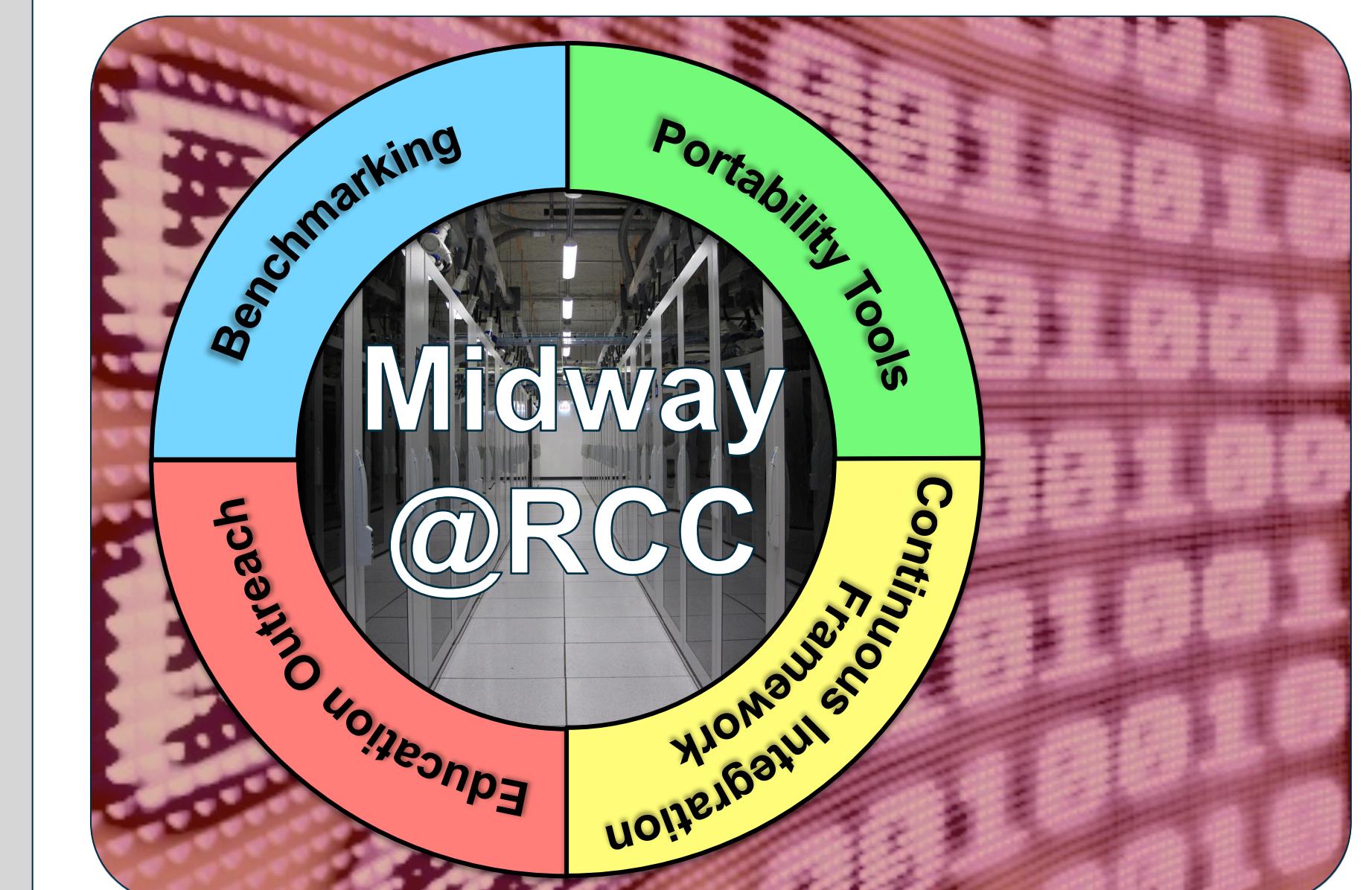


### Energy Storage



### Quantum Information

## Leveraging RCC resources



## Future directions

Apply WEST to interfaces with electrolytes. Explore optical excitations and thermal effects.

Thanks to Early Science Programs at ANL and NERSC we plan to adapt the software to leverage the next generation of HPC machines.

Many integrated cores architectures



## References

- M. Govoni, and G. Galli, *Large scale GW calculations*, J. Chem. Theory Comput. 11, 2680 (2015)
- H. Seo, M. Govoni, and G. Galli, *Design of defect spins in piezoelectric aluminum nitride for solid-state hybrid quantum technologies*, submitted (2015)