Materials discovery and scientific design by computation: what does it take?

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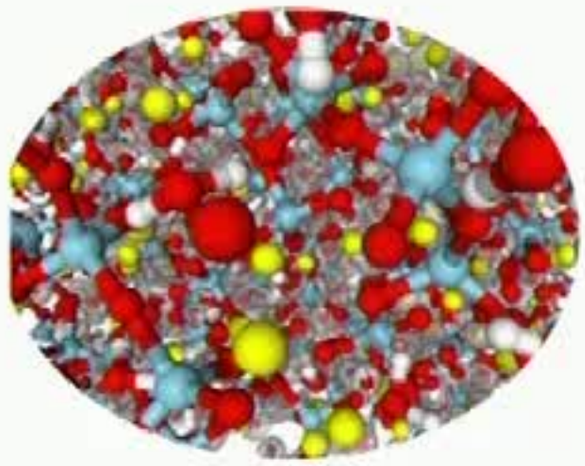
Materials: solids, liquids, nanostructures and combinations thereof



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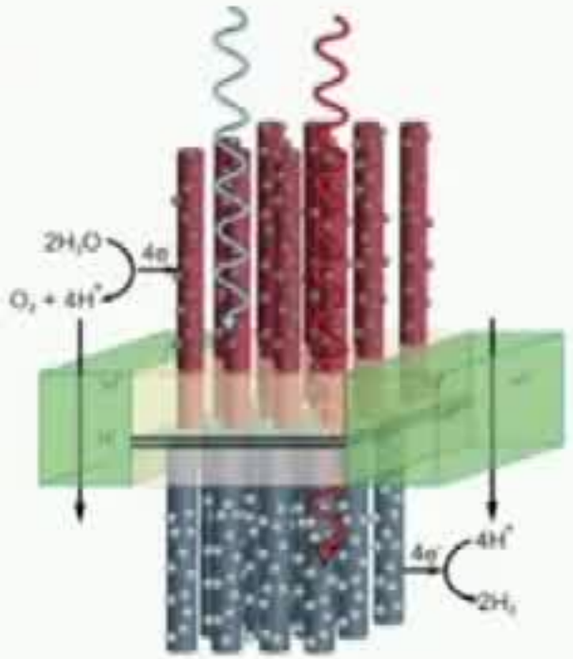
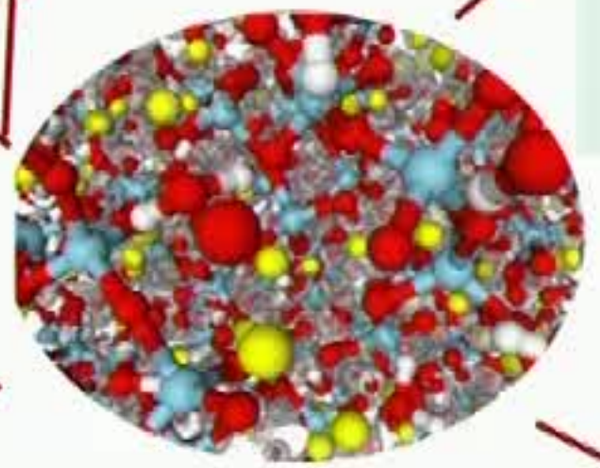
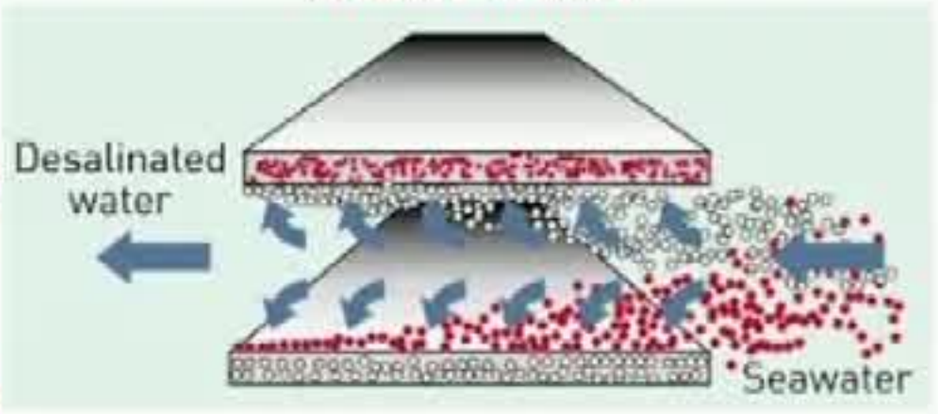
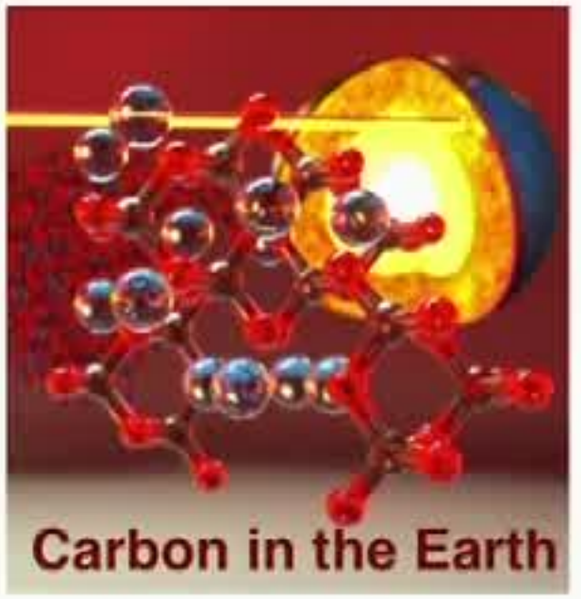


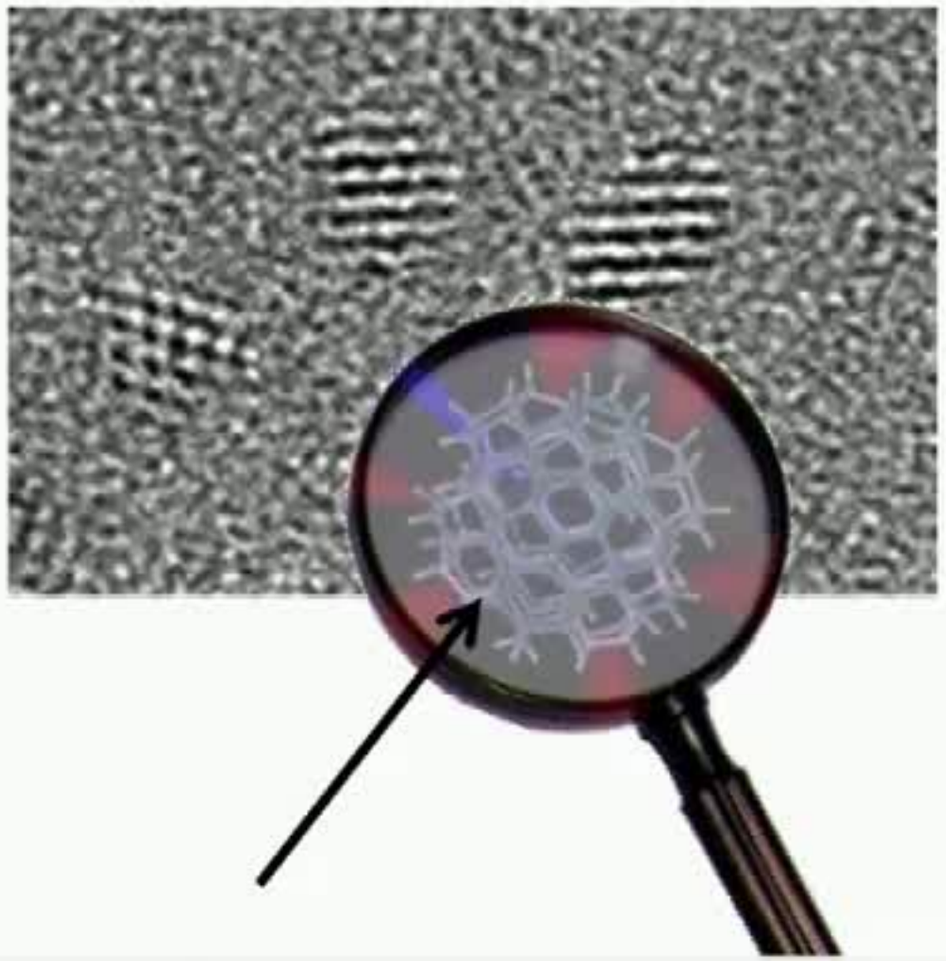
Photo-electrochemical cells







At the microscopic scale



Nuclei: $\{R_I\}_I$

Electrons: $\{\psi_i\}_i$

Materials are complex systems

- Realistic materials are heterogeneous systems
  - —**Understand and control the role of interfaces and defects**

- Discovery and design of materials and emergent behaviors require the ability to compute multiple properties
  - —**Simulations at different length and time scales**

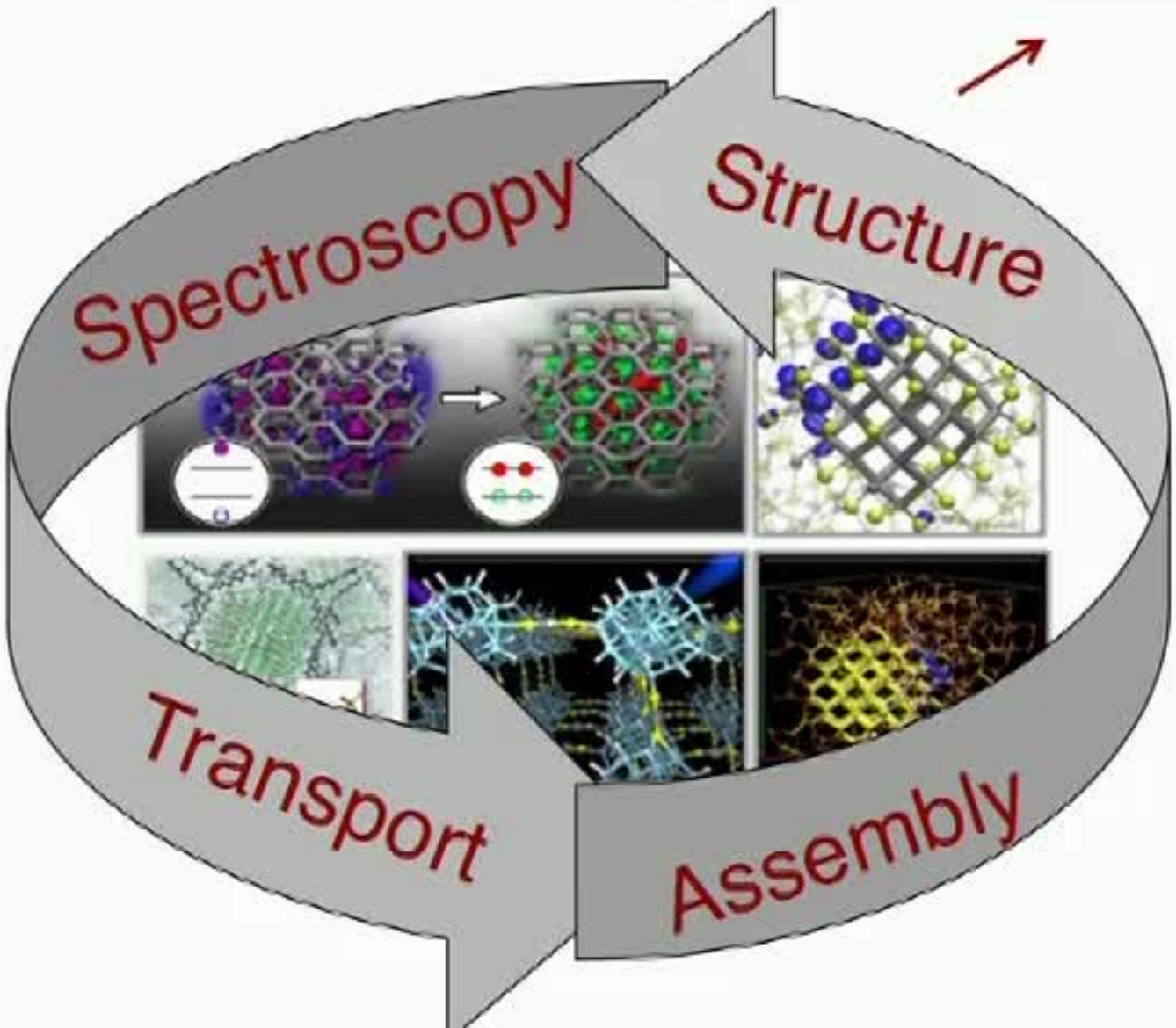
- Desired & new functionalities of materials may arise from assembling building blocks
  - —**Design building blocks with targeted properties and assemble them with precision**

- Desired & new functionalities may arise in metastable systems
  - —**Investigate out of equilibrium processes**
  - —**Simulate assembly processes during synthesis**

Integrated predictions of multiple properties

Integrated predictions of multiple properties

Geometrical arrangements of atoms; thermodynamic properties from approximate solutions of the **Schroedinger equation**



Quantum mechanics: approximations and computation

The approximations:

- **Mean-field theories:** $E_0\left(\{\mathbf{R}_I\}\right) = \mathrm{Min}_{n(\mathbf{r})}\, E_{\{\mathbf{R}\}}\left[n\right]$
  - — **Density Functional Theory** ← ~ 1965
    - – ***Local density approximations*** ← ~ 1985-1990
- **Hartree-Fock and Quantum Chemistry**
- **Stochastic approaches:**
  - — **Quantum Monte Carlo** ← ~ 1980
    - – ***The fixed node approximation***

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The ability to compute:

In the 1990s, Density Functional theory and quantum chemistry are massively used in physics and chemistry, as the results of key algorithmic and computational developments Quantum Monte Carlo is applied to "real materials".

Quantum mechanics: approximations and computation

The approximations:

- **Mean-field theories:** $E_0(\{\mathbf{R}_I\}) = \mathrm{Min}_{n(\mathbf{r})} E_{\{\mathbf{R}\}}[n]$
  - — **Density Functional Theory (DFT)** ← ~ 1965
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Molecular Dynamics (MD) with forces from DFT → ***ab-initio*** **MD**:

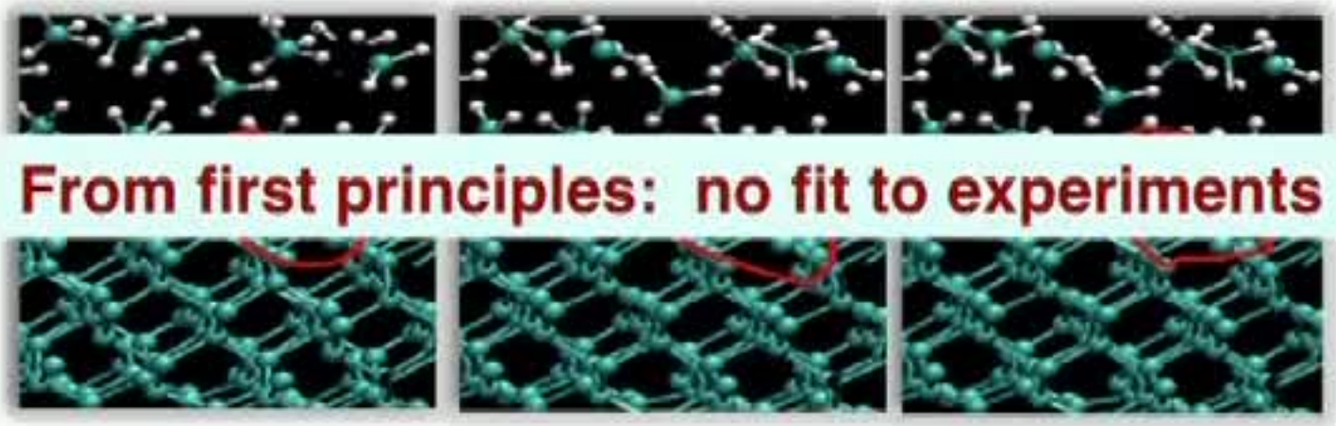
Dynamical and thermodynamic properties from first principles

The ability to compute:

algorithmic and computational developments

- **All-electron solutions to DFT equations**
- ***Ab-initio*** **Molecular Dynamics (Car-Parrinello method)**
- **Linear scaling methods within DFT and QMC**
- **Software development for HPC architectures**

Ab initio Molecular Dynamics



From first principles: no fit to experiments

$$M_I \ddot{R}_I = F_I$$
$$F_I = -\nabla_I \, E(\{R_I(t)\})$$

E **from Density Functional Theory**

Solve set of N coupled, non linear partial differential equations self-consistently, using iterative algorithms, subject to orthonormality constraints. N = # of electrons

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http://qboxcode.org/

Qbox
First-Principles Molecular Dynamics

Complexity of *ab initio* MD: Kohn Sham equations

Solve set of N coupled, non linear partial differential equations self-consistently, using iterative algorithms, subject to orthonormality constraints. N = # of electrons

Condensed Matter Physics

⇕

Physical Chemistry

$$\begin{cases} -\Delta\varphi_i + V(\rho,\mathbf{r})\varphi_i = \varepsilon_i\varphi_i \quad i = 1\ldots N_{\text{el}} \\ V(\rho,\mathbf{r}) = V_{\text{ion}}(\mathbf{r}) + \int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' + V_{\text{XC}}(\rho(\mathbf{r}), \nabla\rho(\mathbf{r})) \\ \rho(\mathbf{r}) = \sum_{i=1}^{N_{\text{el}}} |\varphi_i(\mathbf{r})|^2 \\ \int \varphi_i^*(\mathbf{r})\,\varphi_j(\mathbf{r})\,d\mathbf{r} = \delta_{ij} \end{cases}$$

Hybrid Functionals (*)

The cost of solving the Kohn-Sham equations is eventually dominated by orthogonalization (O(N^3))

(*) J. H. Skone, M. Govoni & GG Phys. Rev. B 2014 & Phys. Rev. B 2016; N. Brawand, M.Voroes, M.Govoni and GG, PRX 2016

Why it is difficult

- Non linear fix-point problem solved using iterative methods to find self-consistent solutions
- For many systems only the lowest invariant subspace is needed (linear combinations of eigenvectors, not individual eigenvectors)
- Full accuracy of eigenvectors and eigenvalues not needed in early stages of self-consistent iterations
- Large basis sets (millions of basis functions)
- Usually tens of thousands of eigenvectors are needed
- Spectrum does not necessarily have a gap and the existence of a gap is not known beforehand
- Cost of matrix-vector product is cubic in the number of electrons

Why using existing eigensolvers is difficult

Existing eigensolvers may be used in inner loops (fixed potential), but:

- Solutions are required at each MD time step (tens of thousands of steps during MD)
- Extrapolation techniques to guess starting point of iterative procedure at the next time step are required
- Number of self-consistent iterations may vary at each MD step
- Threshold for convergence depends on outer loop (specifically, on the value of a functional of eigenvectors)
- Parallel data layout of existing eigensolvers not always compatible with data layout of other parts of the application, implying substantial data transfer

Existing eigensolvers (Scalapack, ELPA) are used to solve the Ritz problem, once the invariant subspace has been determined

Some examples

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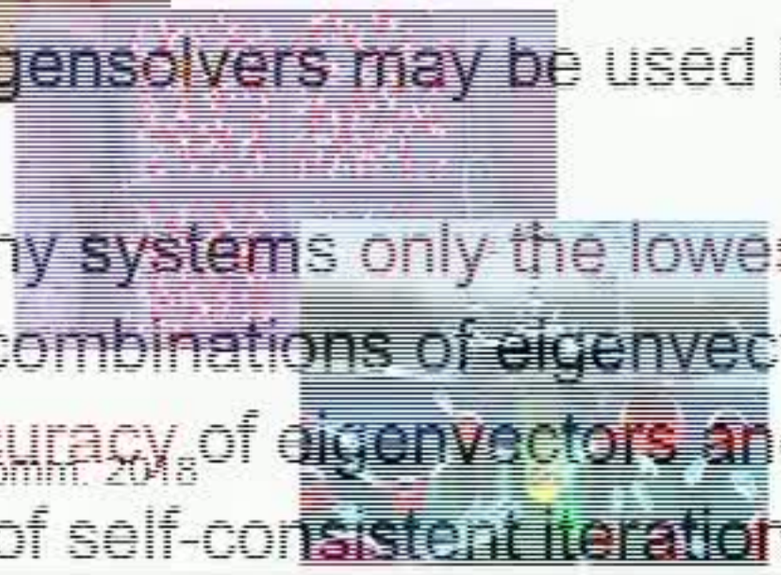

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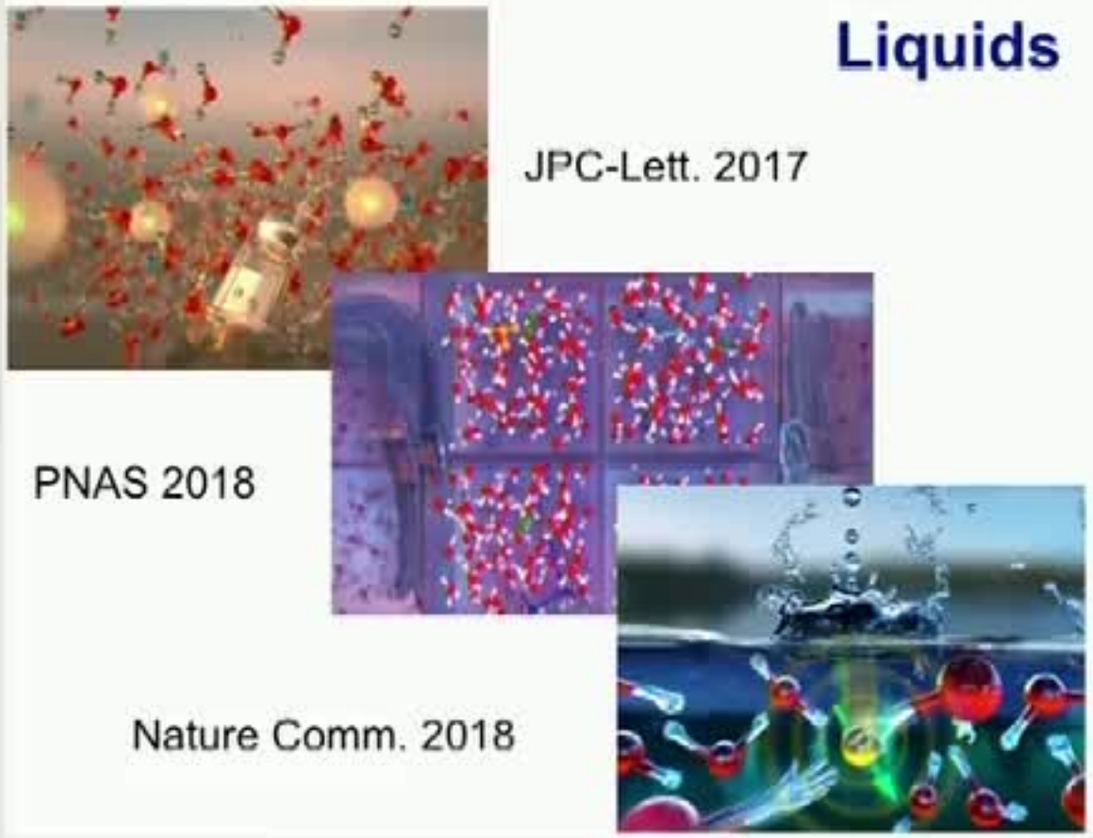
Liquids

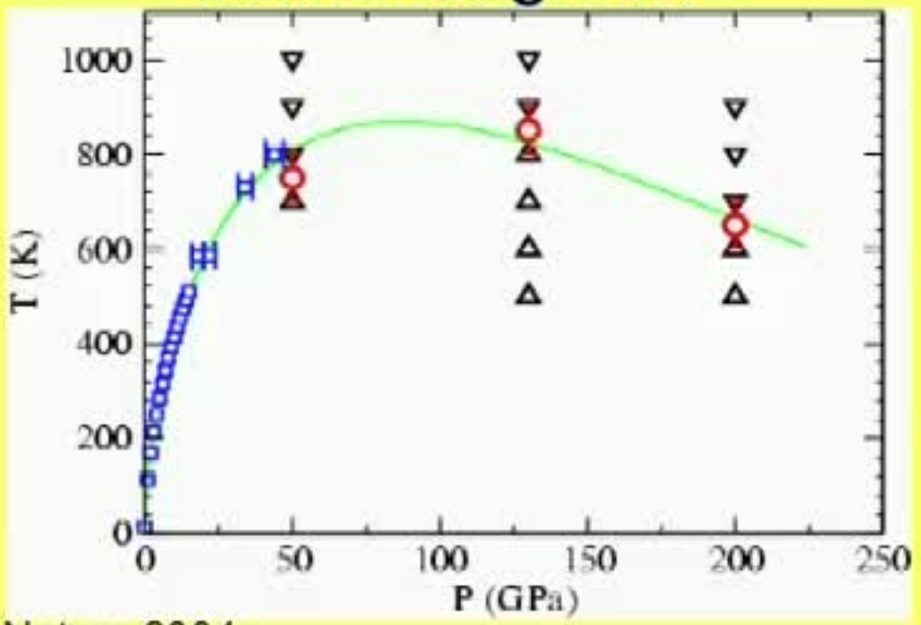


JPC-Lett. 2017

PNAS 2018

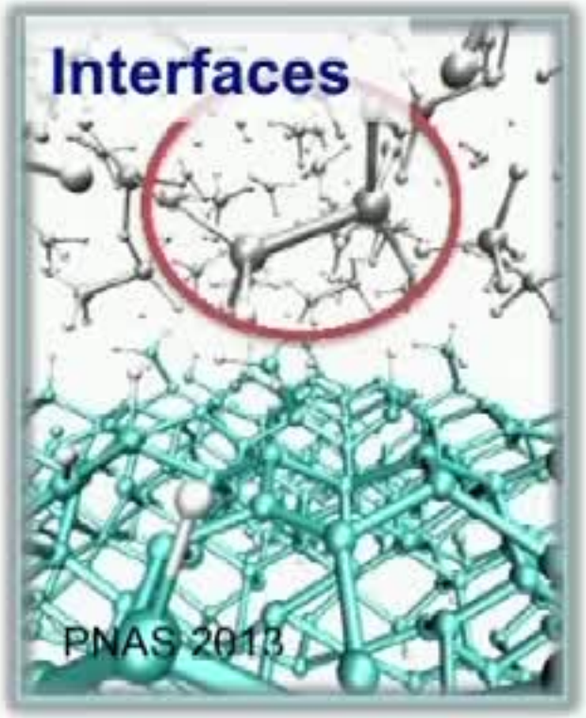
Nature Comm. 2018

Phase diagrams



Nature 2004

Interfaces



PNAS 2013

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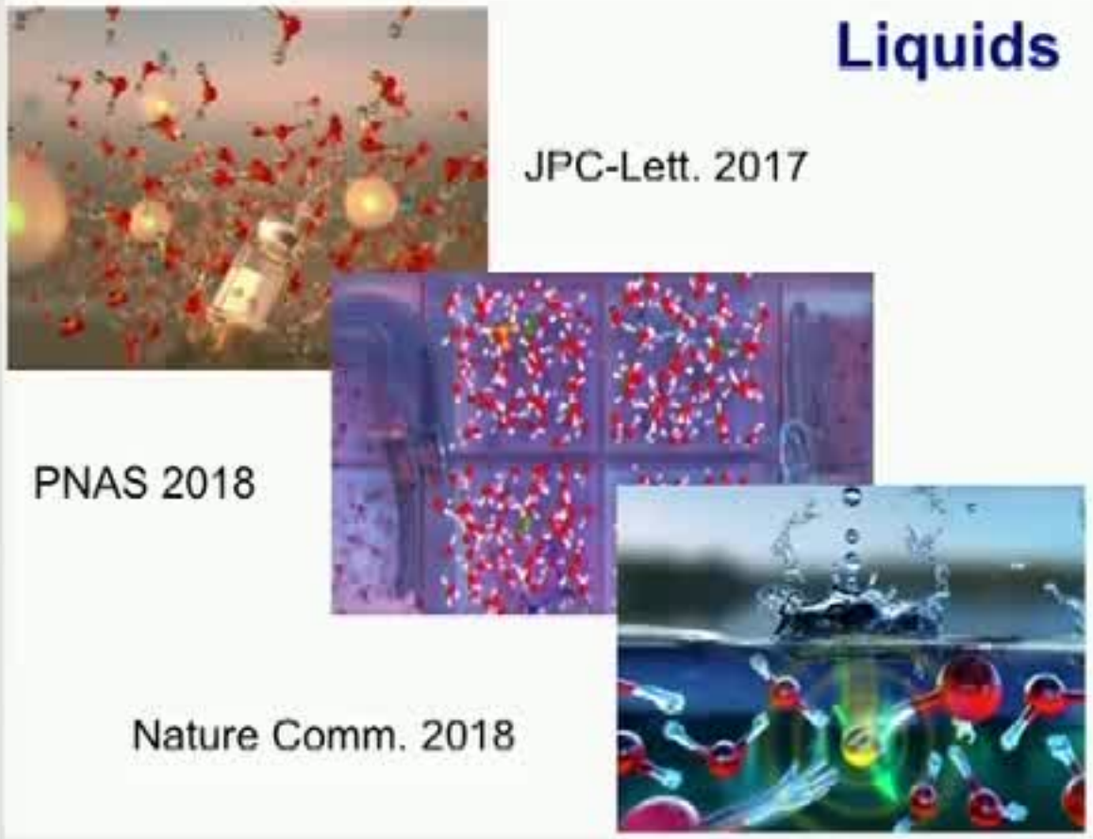
Liquids



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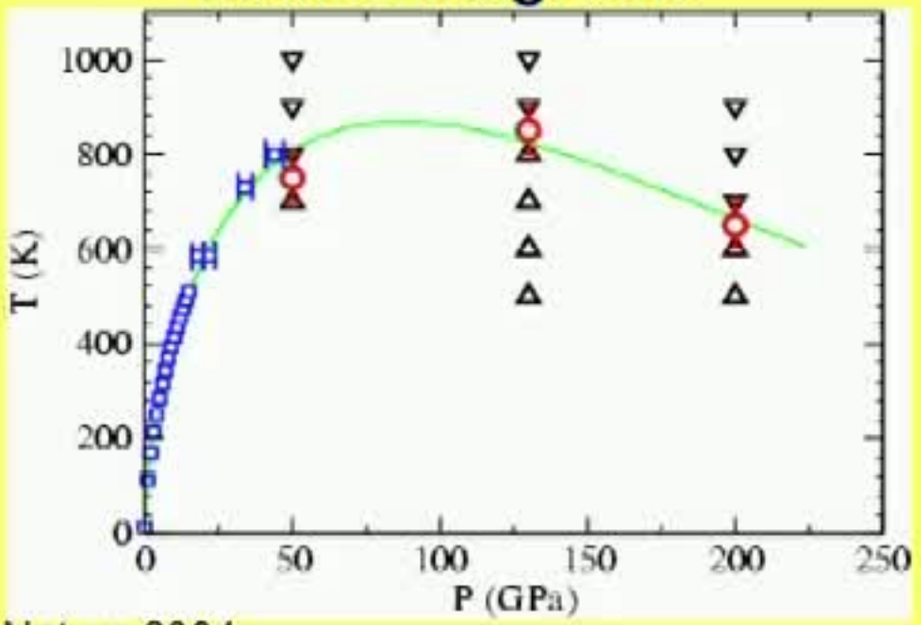

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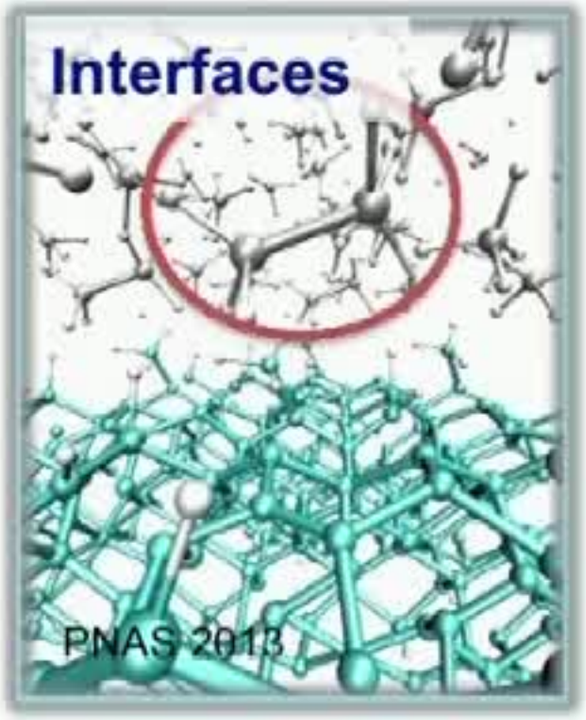


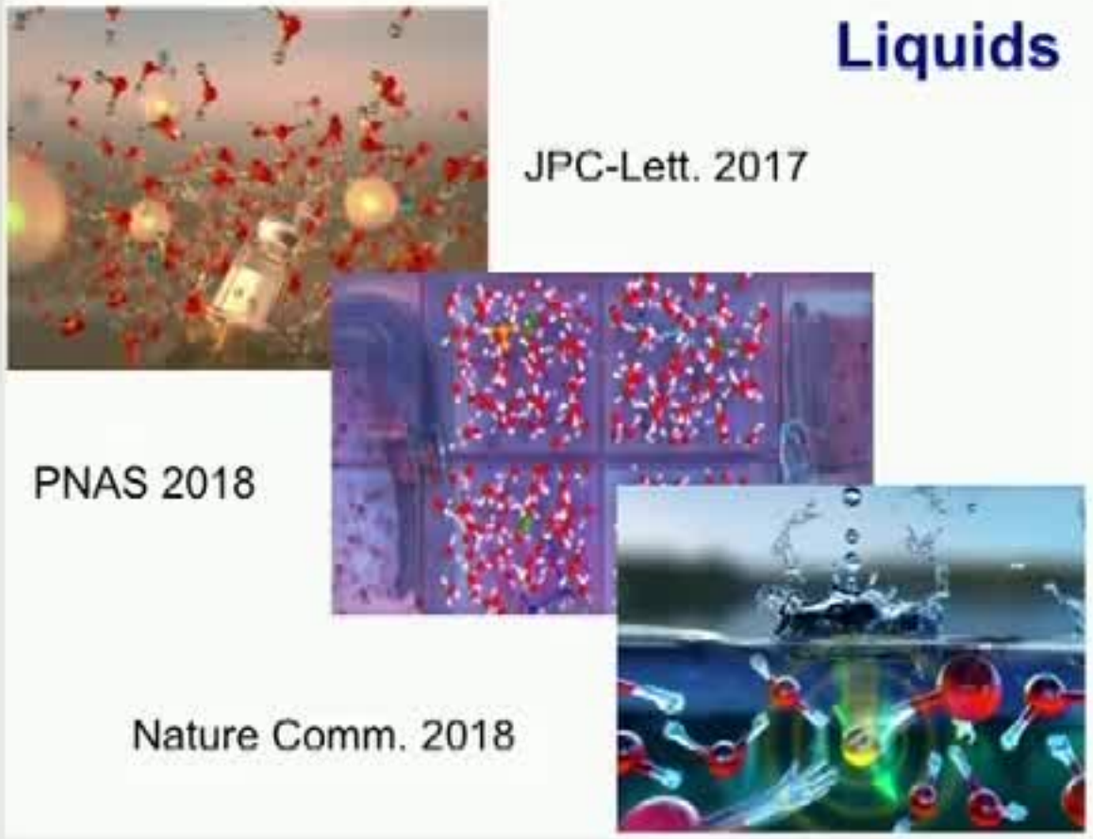
PNAS 2013

Defects in solids

Nature Comm. 2016

Some examples

Liquids



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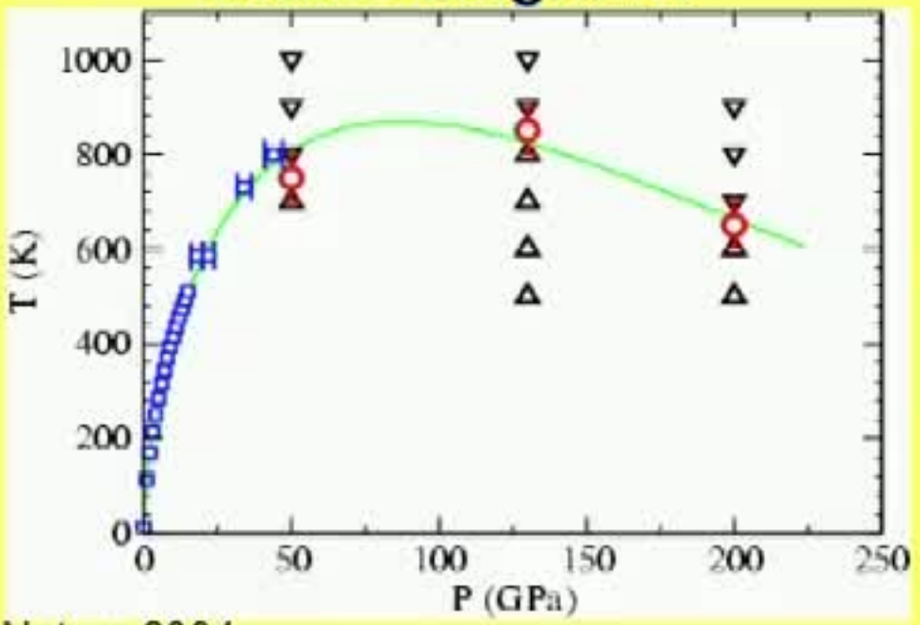

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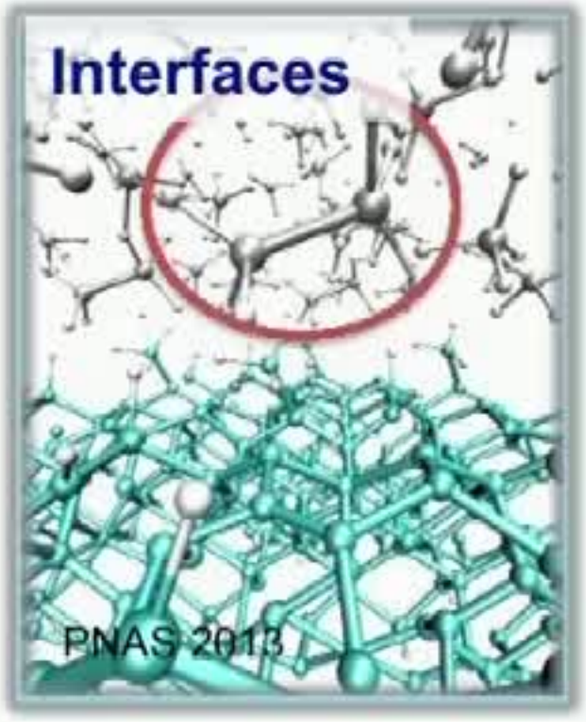

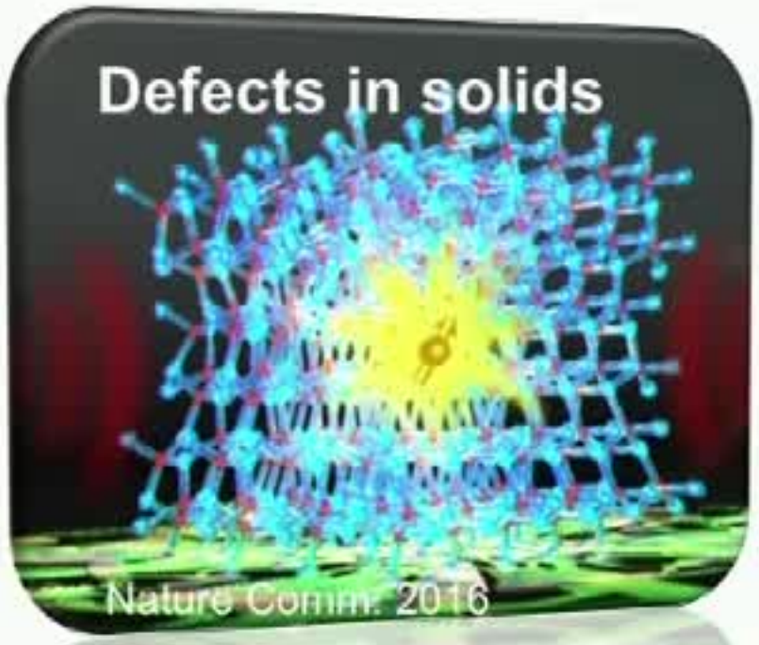

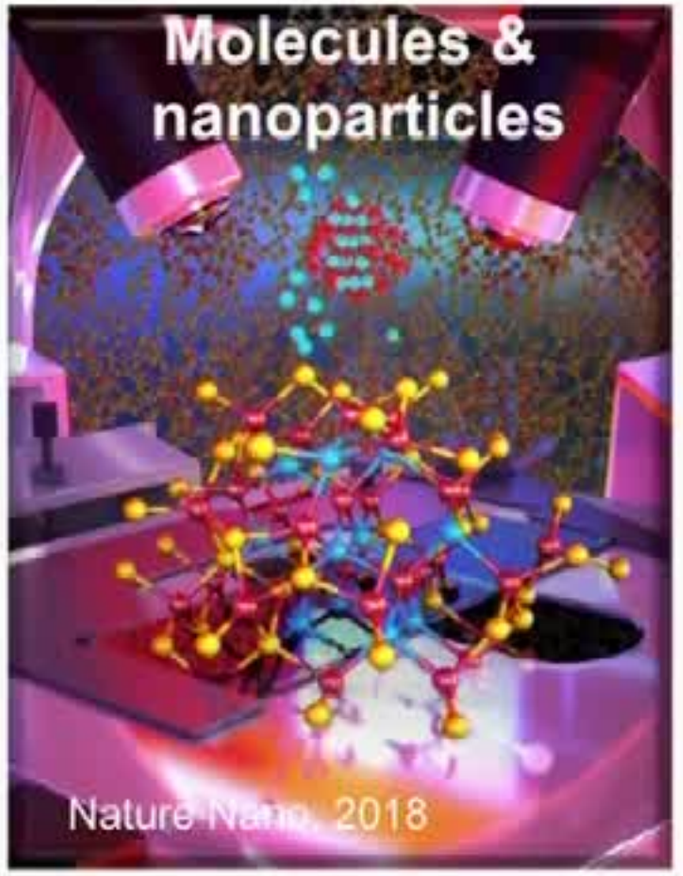

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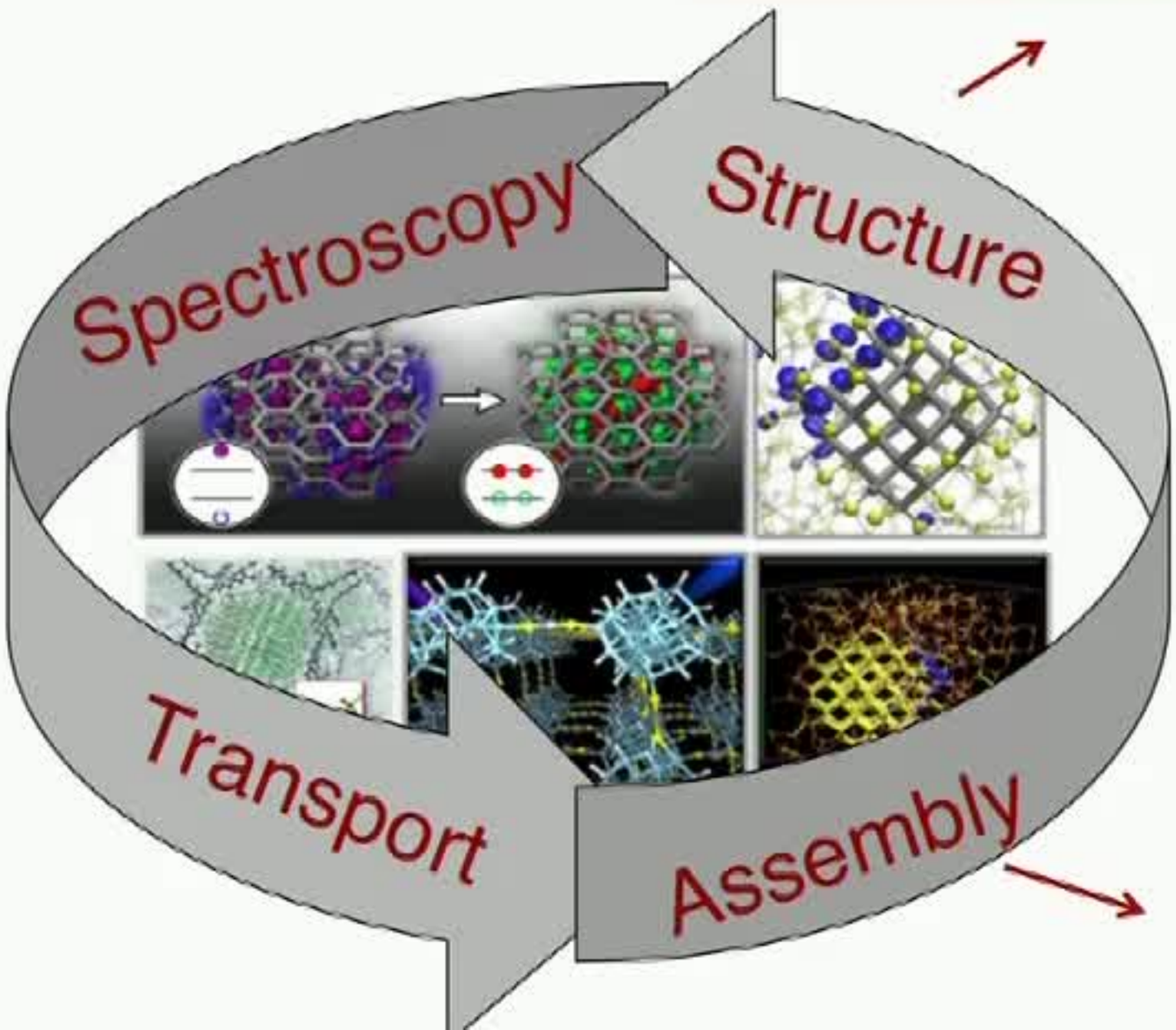
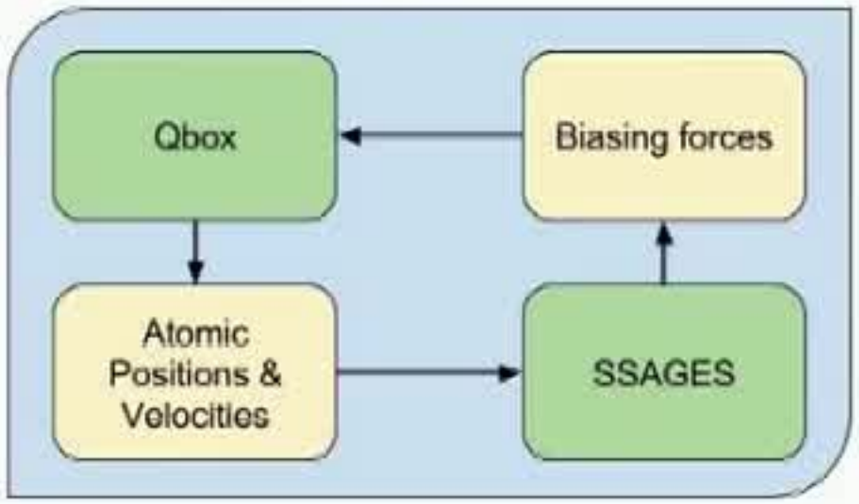


Advanced sampling techniques to assemble components/ constituents out of equilibrium

Advanced sampling and ab initio MD

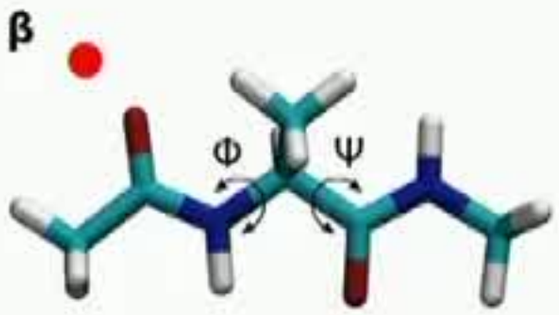


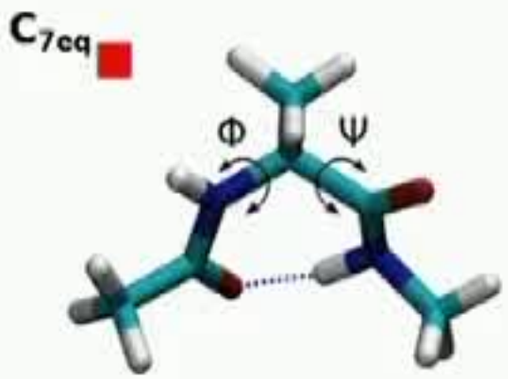
Qbox-SSAGES: Advanced sampling coupled with first-principles MD with DFT and hybrid DFT

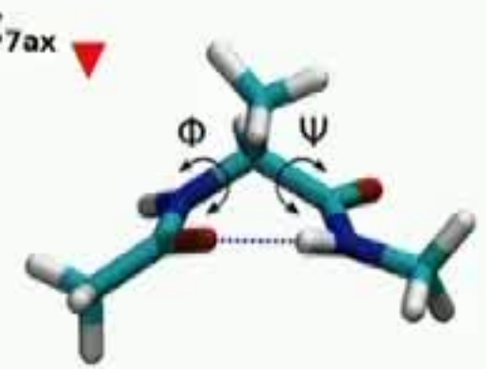
Whitmer-Gygi-de Pablo-Galli collaboration
JCTC 2018

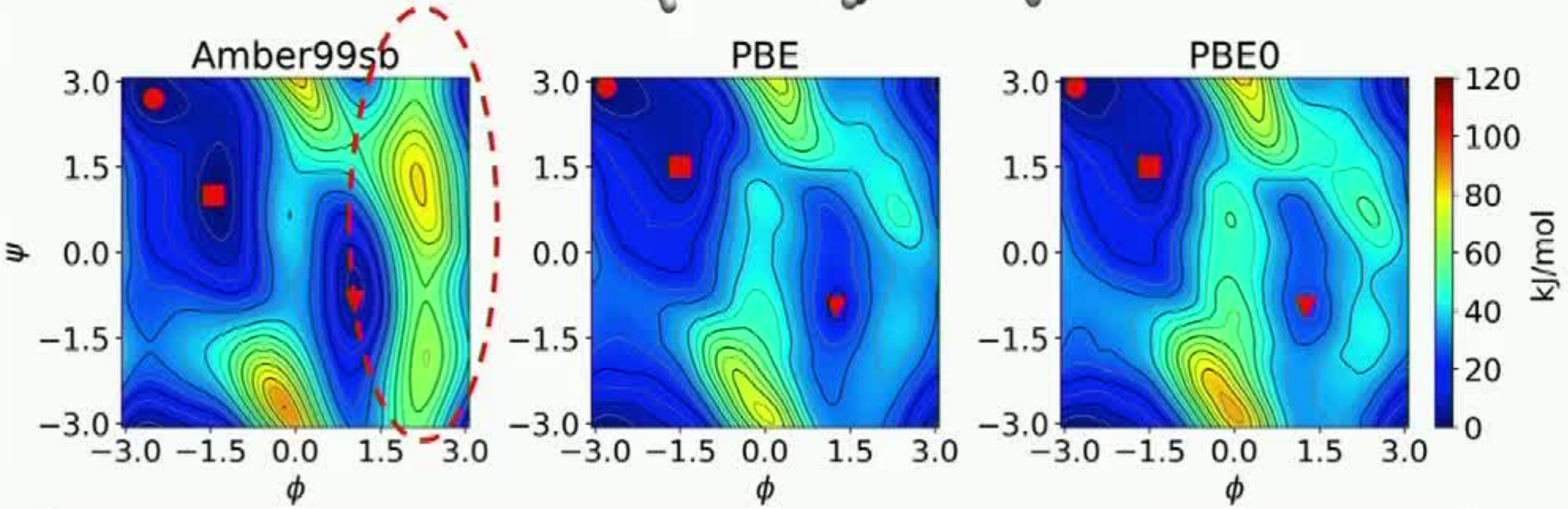
The coupled Qbox- SSAGES framework permits a hierarchical coupling. High level of theory (hybrid-functional) calculations can be restarted from previously converged lower level of theory (GGA) calculations.

Free energy calculations of a peptide





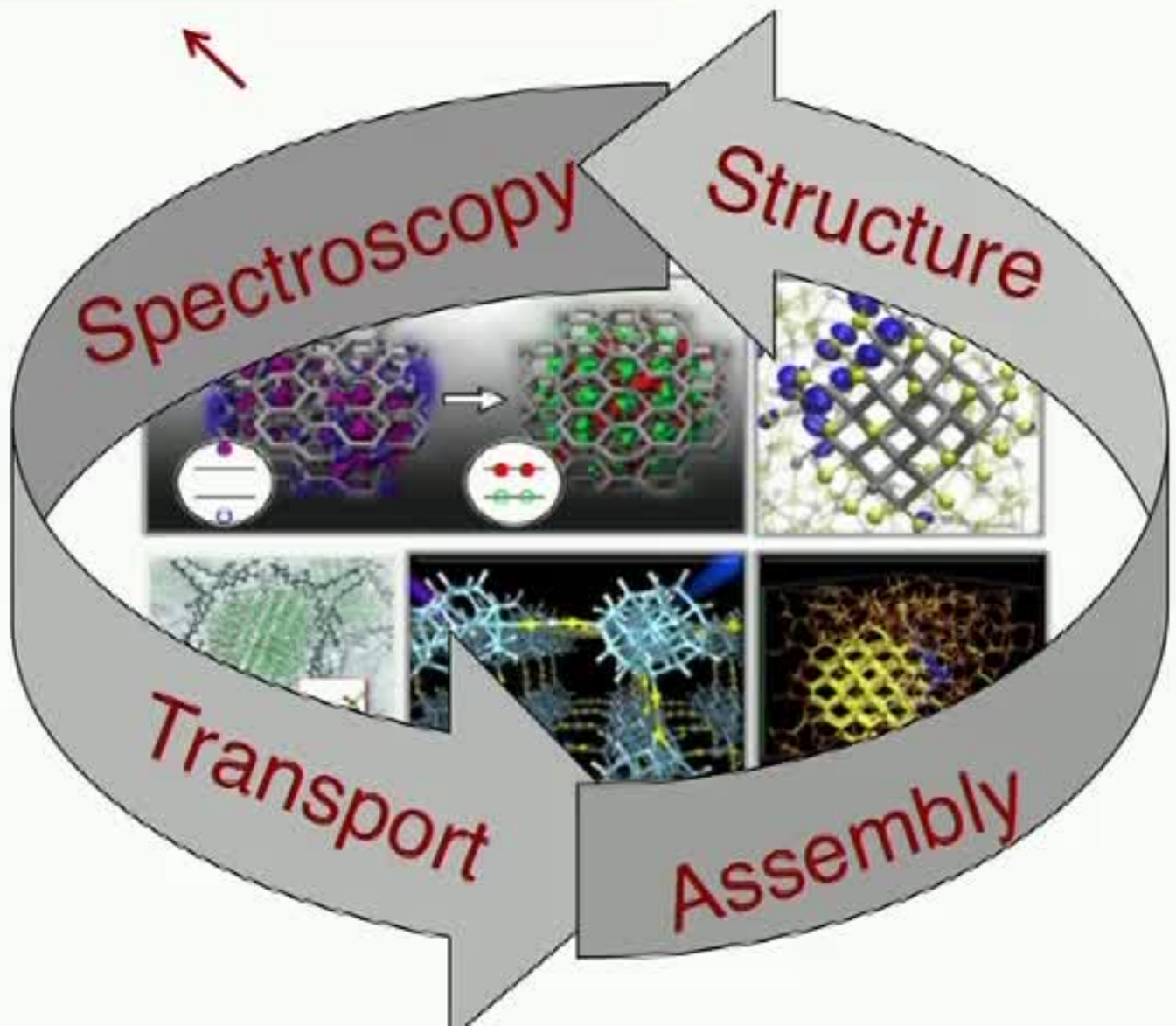




Significant deviation in the free energy surfaces obtained at the DFT level (PBE and PBE0) from that calculated with **Amber99sb**

Integrated predictions of multiple properties

Interaction with electromagnetic fields (light) from the **coupling of Maxwell and Schroedinger equations** using linear response and perturbation theory



Spectroscopy on "MD samples"

Use trajectories to compute complex electronic properties from **many body perturbation (MBPT)** theory → Electronic properties at finite T w/statistical errors

$$\left(\hat{T} + \hat{V}_{ion} + \hat{V}_H + \hat{V}_{xc}\right)|\psi_n\rangle = \varepsilon_n |\psi_n\rangle \qquad \text{DFT}$$

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

H. Wilson, F. Gygi, and G. G., PRB 2008; H.Wilson, D.Lu, F.Gygi and G.G., Phys.Rev.B 2009
H. V. Nguyen, T.A. Pham, D.Rocca and GG Phys. Rev. B (R) 2012; T.A.Pham, H.V.Nguyen, D.Rocca and GG, Phys.Rev.B 2013
M.Govoni & GG, J. Chem. Theory Comput., (2015); P.Scherpelz, I.Hamada, M.Govoni and GG, JCTC (2017); M.Govoni and GG, JCTC 2018

Maxwell equations for the external field

- D = E + 4πP D = external field, independent of the material

$$\nabla \cdot \mathbf{D} = 4\pi Q n_{\text{ext}} \qquad \nabla \times \mathbf{E}(t) = -\frac{1}{c}\frac{\mathrm{d}\mathbf{B}}{\mathrm{d}t}$$

$$\nabla \cdot \mathbf{B} = 0 \qquad \nabla \times \mathbf{B}(t) = \frac{4\pi}{c}\mathbf{j}_{\text{ext}} + \frac{1}{c}\frac{\mathrm{d}\mathbf{D}}{\mathrm{d}t}$$

- Relation between current and total field and density and total field

$$\mathbf{j}_{\text{int}}(\mathbf{r},t) = \int \mathrm{d}\mathbf{r}' \int^{t} \sigma(\mathbf{r},\mathbf{r}',t-t')\mathbf{E}(\mathbf{r}',t')$$

$$\mathbf{j}_{\text{int}}(\mathbf{r},\omega) = \int \mathrm{d}\mathbf{r}'\sigma(\mathbf{r},\mathbf{r}',\omega)\mathbf{E}(\mathbf{r}',\omega)$$

$$\mathbf{D}(\mathbf{r},\omega) = \int \mathrm{d}\mathbf{r}'\epsilon(\mathbf{r},\mathbf{r}',\omega)\mathbf{E}(\mathbf{r}',\omega)$$

$$\mathbf{E}(\mathbf{r},\omega) = \int \mathrm{d}\mathbf{r}'\epsilon^{-1}(\mathbf{r},\mathbf{r}',\omega)\mathbf{D}(\mathbf{r}',\omega)$$

- Response to the total field E

$$\epsilon(\mathbf{r},\mathbf{r}',\omega) = \mathbf{1}\delta(\mathbf{r}-\mathbf{r}') + \frac{4\pi i}{\omega}\sigma(\mathbf{r},\mathbf{r}',\omega)$$

- Response to the external field D → $\epsilon^{-1}(\mathbf{r},\mathbf{r}',\omega)$

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

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Hedin equations

Hedin proposed to express Σ in terms of the **dynamically screened Coulomb potential**, instead of the bare Coulomb potential

$$\left(\hat{T}+\hat{V}_{ion}+\hat{V}_H+\hat{V}_{xc}\right)|\psi_n\rangle=\varepsilon_n|\psi_n\rangle \quad \text{DFT}$$

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

$$\Sigma(\mathbf{r},\mathbf{r}';\omega)=\int\frac{d\omega}{2\pi}G(\mathbf{r},\mathbf{r}';\omega+\omega')W(\mathbf{r},\mathbf{r}';\omega')$$

$$G(\mathbf{r},\mathbf{r}';\omega)=\langle\mathbf{r}|\frac{1}{\omega-H}|\mathbf{r}'\rangle$$

$$W(\mathbf{r},\mathbf{r}';\omega)=\int d\mathbf{r}''\,\epsilon^{-1}(\mathbf{r},\mathbf{r}'';\omega)v_c(\mathbf{r}'',\mathbf{r}')$$

Use an expression in terms of Kohn-Sham electronic states from density-density response functions

$$E_n^{QP}=\varepsilon_n^{KS}+\left\langle\psi_n^{KS}\middle|\,\hat{\Sigma}(E_n^{QP})-\hat{V}_{xc}\,\middle|\psi_n^{KS}\right\rangle$$

L. Hedin, Phys. Rev. 139, A796 (1965)

Calculations of dielectric matrices: spectral decomposition & DFPT

$$\tilde{\epsilon}^{-1} = \sum_{i=1}^{\text{Neig}} \tilde{\phi}_i \left(\frac{\lambda_i}{1-\lambda_i} + 1 \right) \tilde{\phi}_i^H$$

- Calculation of empty electronic states, calculation and storage of full dieletric matrix and inversion of $\tilde{\epsilon}$ are avoided
- Scaling: $N_{eig} N_{pw} N_v^2$ (instead of $N_{pw}^2 N_v N_c$)
- Efficient evaluation of $\tilde{\epsilon}^{-1}$ at different **q** points and at different MD steps is possible
- Incorporation of XC kernel is in principle straightforward

H. Wilson, F. Gygi, and G. G., PRB 2008; H.Wilson, D.Lu, F.Gygi and G.G., Phys.Rev.B 2009; V. H. Nguyen, S. de Gironcoli, Phys.Rev.B 2009, M.Govoni & GG, J. Chem. Theory Comput., (2015)

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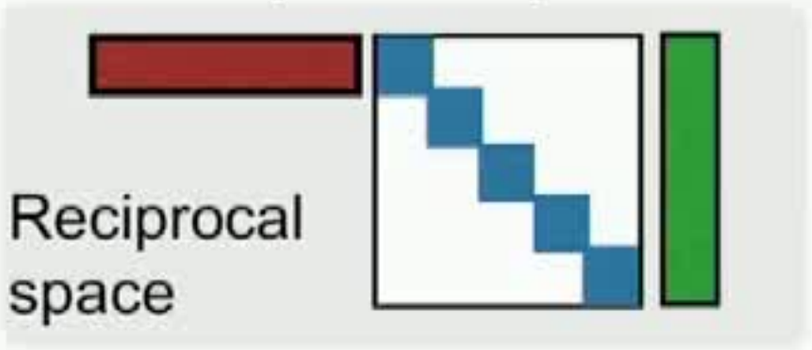
- Incorporation of XC kernel is in principle straightforward

H. Wilson, F. Gygi, and G. G., PRB 2008; H.Wilson, D.Lu, F.Gygi and G.G., Phys.Rev.B 2009; V. H. Nguyen, S. de Gironcoli, Phys.Rev.B 2009, M.Govoni & GG, J. Chem. Theory Comput., (2015)

Low rank decomposition of the screened Coulomb interaction W

In **Hartree-Fock**

$$\langle \psi_i \psi_j | \frac{1}{|\mathbf{r} - \mathbf{r}'|} | \psi_k \psi_l \rangle$$



In **GW**

$$\langle \psi_i \psi_j | W(\mathbf{r}, \mathbf{r}') | \psi_k \psi_l \rangle$$

$$W = \sum_{\alpha} |\alpha\rangle \lambda_\alpha \langle \alpha|$$ **Low-rank decomposition**

Separable form

Calculations of dielectric matrices: spectral decomposition & DFPT

$$\tilde{\epsilon}^{-1} = \sum_{i=1}^{\text{Neig}} \tilde{\phi}_i \left(\frac{\lambda_i}{1-\lambda_i} + 1 \right) \tilde{\phi}_i^H$$

- Calculation of empty electronic states, calculation and storage of full dieletric matrix and inversion of $\tilde{\epsilon}$ are avoided
- Scaling: $N_{eig} N_{pw} N_v^2$ (instead of $N_{pw}^2 N_v N_c$)
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Hedin equations

Hedin proposed to express Σ in terms of the **dynamically screened Coulomb potential**, instead of the bare Coulomb potential

$$\left(\hat{T}+\hat{V}_{ion}+\hat{V}_H+\hat{V}_{xc}\right)|\psi_n\rangle=\varepsilon_n|\psi_n\rangle \quad \text{DFT}$$

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

$$\Sigma(\mathbf{r},\mathbf{r}';\omega)=\int\frac{d\omega}{2\pi}G(\mathbf{r},\mathbf{r}';\omega+\omega')W(\mathbf{r},\mathbf{r}';\omega')$$

$$G(\mathbf{r},\mathbf{r}';\omega)=\langle\mathbf{r}|\frac{1}{\omega-H}|\mathbf{r}'\rangle$$

$$W(\mathbf{r},\mathbf{r}';\omega)=\int d\mathbf{r}''\,\epsilon^{-1}(\mathbf{r},\mathbf{r}'';\omega)v_c(\mathbf{r}'',\mathbf{r}')$$

Use an expression in terms of Kohn-Sham electronic states from density-density response functions

$$E_n^{QP}=\varepsilon_n^{KS}+\left\langle\psi_n^{KS}\middle|\,\hat{\Sigma}(E_n^{QP})-\hat{V}_{xc}\,\middle|\psi_n^{KS}\right\rangle$$

L. Hedin, Phys. Rev. 139, A796 (1965)

Calculations of dielectric matrices: spectral decomposition & DFPT

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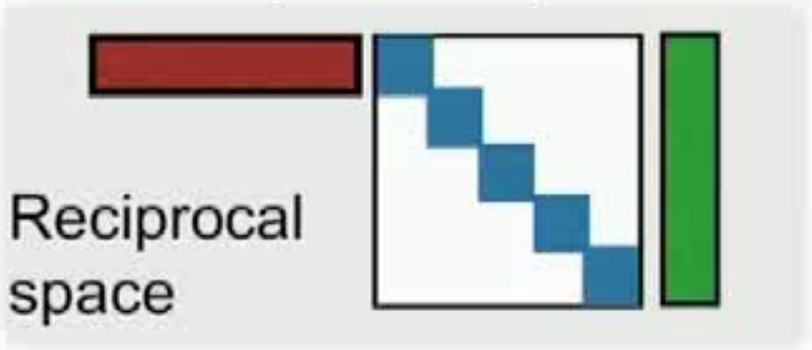

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Separable form

Low rank decomposition of the screened Coulomb interaction W

In **Hartree-Fock**

$$\langle \psi_i \psi_j | \frac{1}{|\mathbf{r}-\mathbf{r}'|} | \psi_k \psi_l \rangle$$

Example : 64 water molecules

Direct space	size~$(250)^3$ x $(250)^3$
	Difficult to truncate
Reciprocal space	size~(1'000'000) x (1'000'000)
	Could be truncated, full matrix
Eigenpotential space	size~(1'000) x (1'000)

In **GW**

$$\langle \psi_i \psi_j | W(\mathbf{r},\mathbf{r}') | \psi_k \psi_l \rangle$$

$$W = \sum_{\alpha} |\alpha\rangle \lambda_\alpha \langle \alpha|$$ **Low-rank decomposition**

Separable form

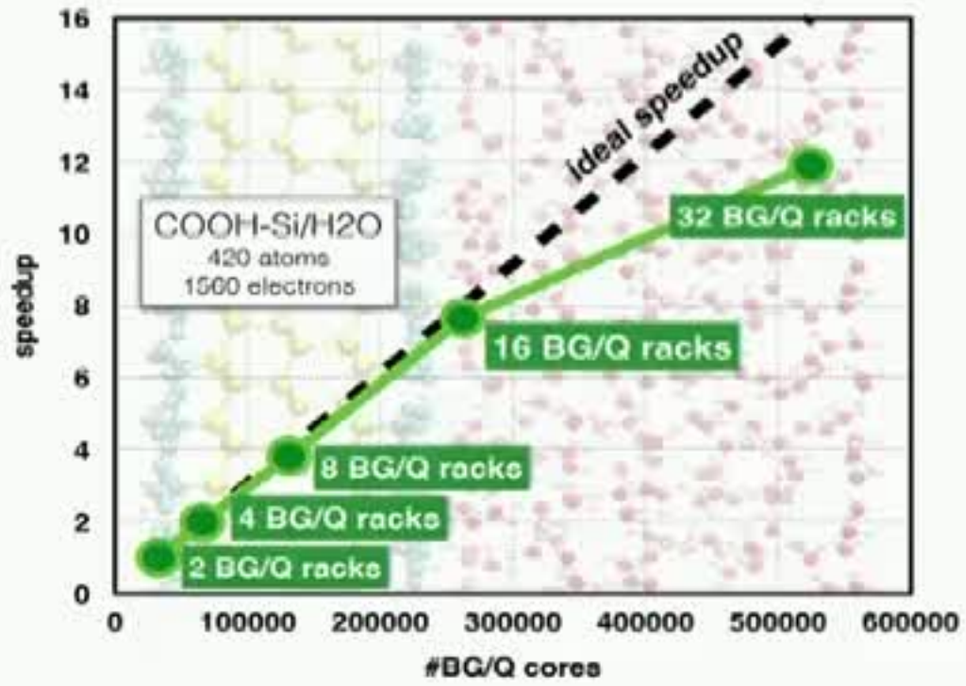
Summary of GW algorithm

- Iterative diagonalization of the dielectric matrix (+) →
- Low rank decomposition of W
- DFPT (*) based projection techniques to compute G
- Eigenpotentials of $\tilde{\epsilon}$ as basis set also at finite frequency (++)
- Lanczos algorithm to compute frequency dependence of dielectric matrix in parallel
- Contour deformation technique for frequency integration (&)

(*) S. Baroni, et al., Rev. Mod. Phys., 73:515, 2001.

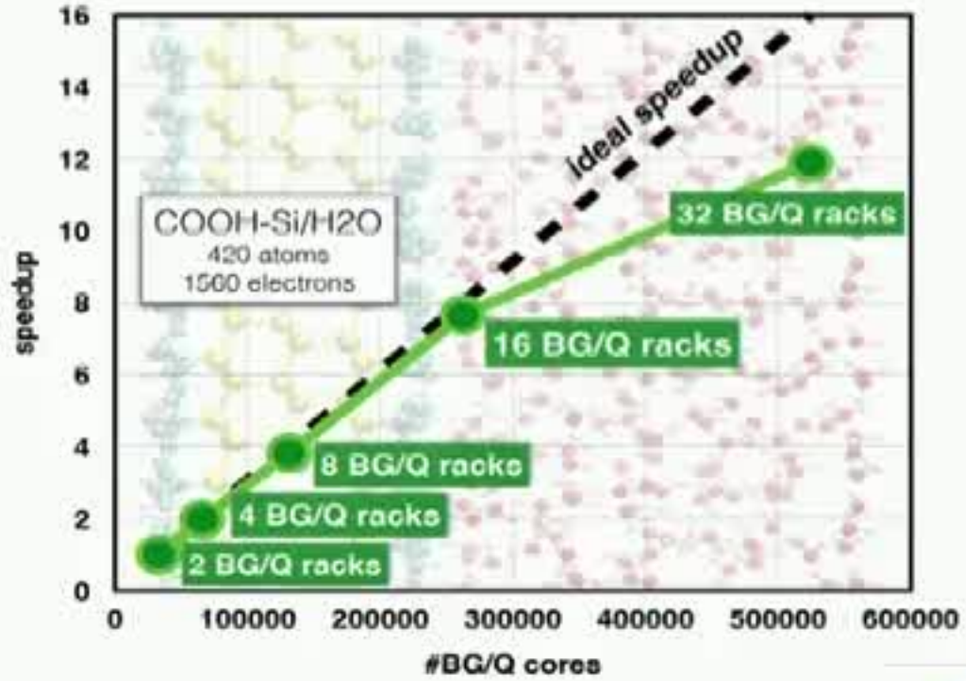
(+) H. Wilson, F. Gygi, and G. G., PRB 2008; H.Wilson, D.Lu, F.Gygi and G.G., Phys.Rev.B 2009
(++) H. V. Nguyen, T.A. Pham, D.Rocca and GG Phys. Rev. B (R) 2012; T.A.Pham, H,V.Nguyen, D.Rocca and GG, Phys.Rev.B 2013
(&) M.Govoni & GG, J. Chem. Theory Comput., (2015)

Implementation of GW algorithm



- Eliminated summations over **empty states** using DFPT
- W made **separable** using the eigenvectors of the dielectric matrix as basis set; number of eigenpotentials controls the **accuracy** of the method.
- Greatly reduced **pre-factors** of $O(N^4)$ scaling

Implementation of GW algorithm



Range of applicability

Ordered and disordered solids, defective materials, liquids, molecular crystals, nanostructures, interfaces

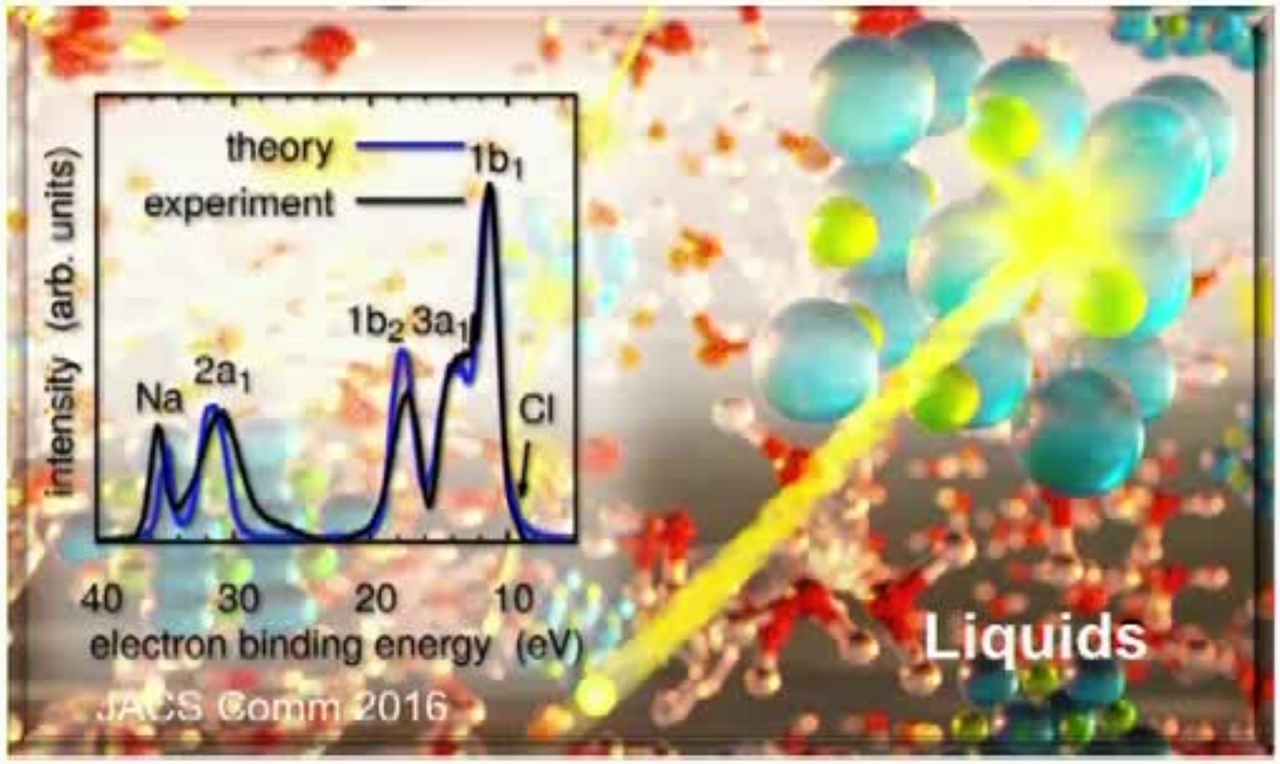
Govoni&GG, JCTC 2015, JCTC 2018

www.west-code.org

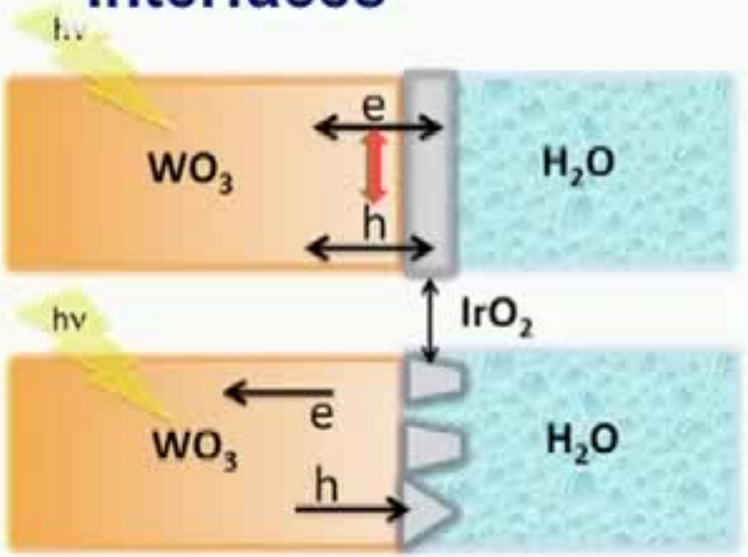
scalable to > 500,000 cores

- Eliminated summations over **empty states** using DFPT
- W made **separable** using the eigenvectors of the dielectric matrix as basis set; number of eigenpotentials controls the **accuracy** of the method.
- Greatly reduced **pre-factors** of $O(N^4)$ scaling

Some examples

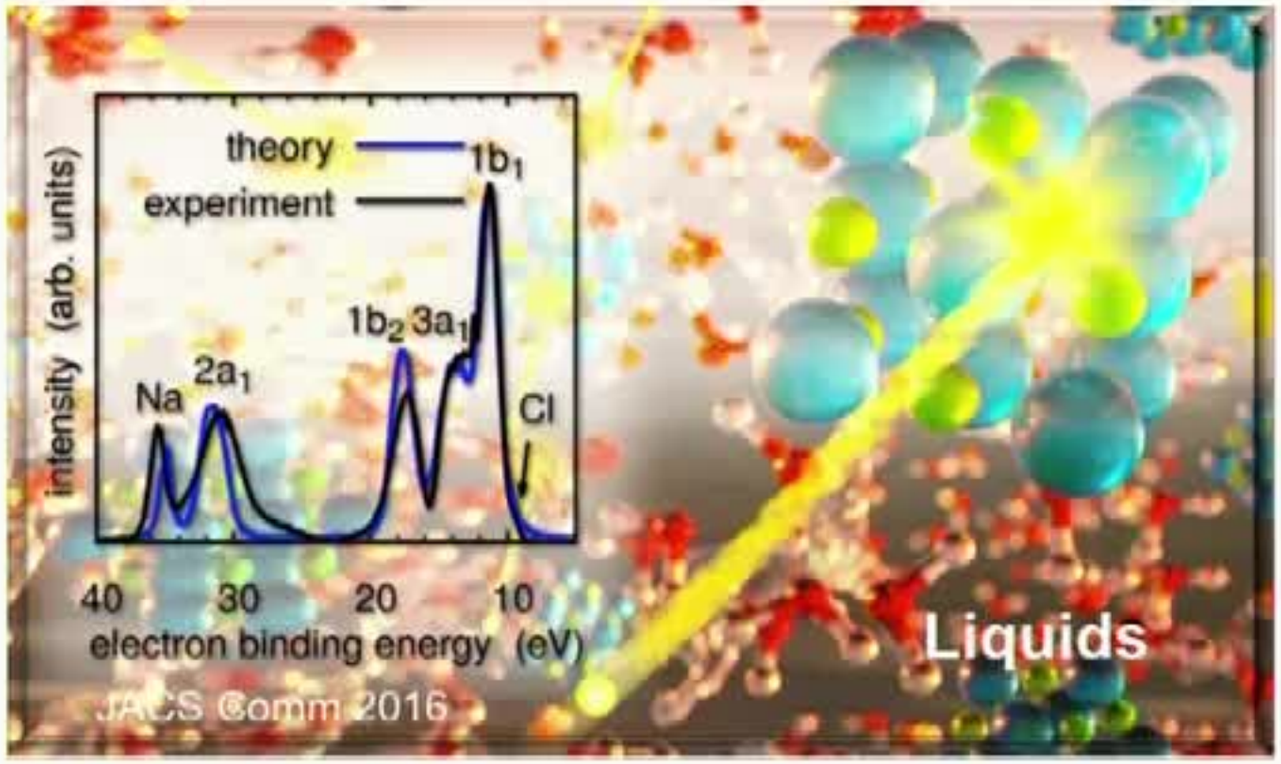


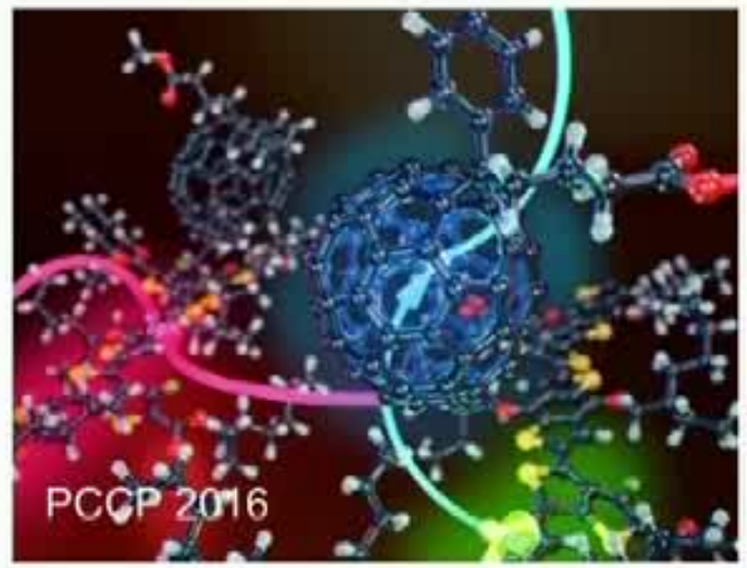
Interfaces



JACS Comm 2015

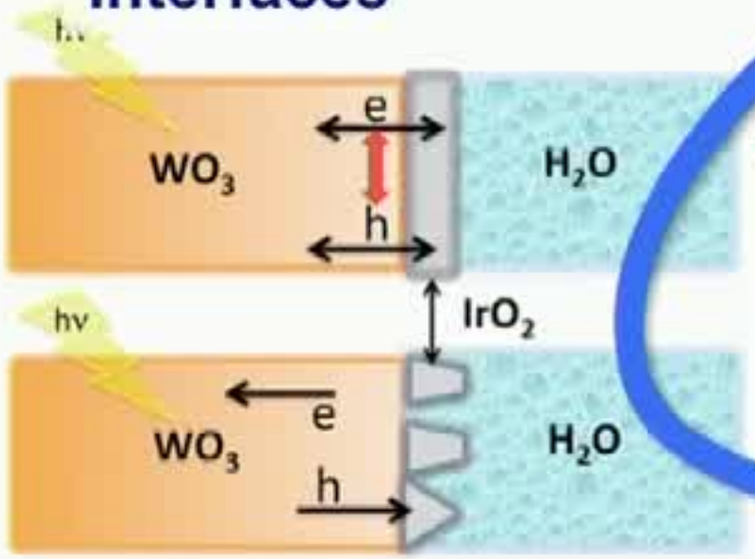
Some examples





Nanoparticles

Interfaces



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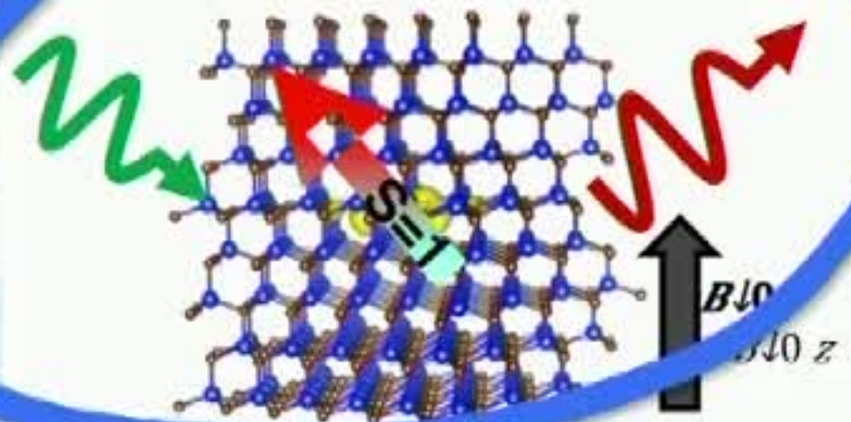
Defects in solids



Nature Comm. 2016

Absorption of light: solving the Bethe Salpeter equation (BSE)

Quantum Liouville equation

$$i\frac{d\hat{\rho}(t)}{dt} = \left[\hat{H}(t), \hat{\rho}(t)\right]$$

$$\hat{H}(t)\phi(\mathbf{r},t) = \left[-\frac{1}{2}\nabla^2 + v_H(\mathbf{r},t) + v_{ext}(\mathbf{r},t)\right]\phi(\mathbf{r},t) + \int \Sigma(\mathbf{r},\mathbf{r}',t)\phi(\mathbf{r}',t)d\mathbf{r}'$$

$$\Sigma_{COH}(\mathbf{r},\mathbf{r}') = \frac{1}{2}\delta(\mathbf{r}-\mathbf{r}')W_p(\mathbf{r}',\mathbf{r}) \qquad \text{BSE}$$

$$\Sigma_{SEX}(\mathbf{r},\mathbf{r}',t) = -\sum_v \phi_v(\mathbf{r},t)\phi_v^*(\mathbf{r}',t)W(\mathbf{r}',\mathbf{r})$$

Screened Coulomb interaction

- The quantum Liouville equation is solved within linear response theory
- Explicit calculation of empty electronic states is avoided by using iterative diag. of ε
- The Tamm-Dancoff approximation is not necessary

D. Rocca, D. Lu, and G. Galli, *JCP* (2010)
D. Rocca, Y. Ping, R. Gebauer, and G. Galli, PRB (2012)

D. Rocca, R. Gebauer, Y. Saad, and S. Baroni, *JCP* (2008)
B. Walker, R. Gebauer, A. M. Saitta, and S. Baroni, PRL (2006)

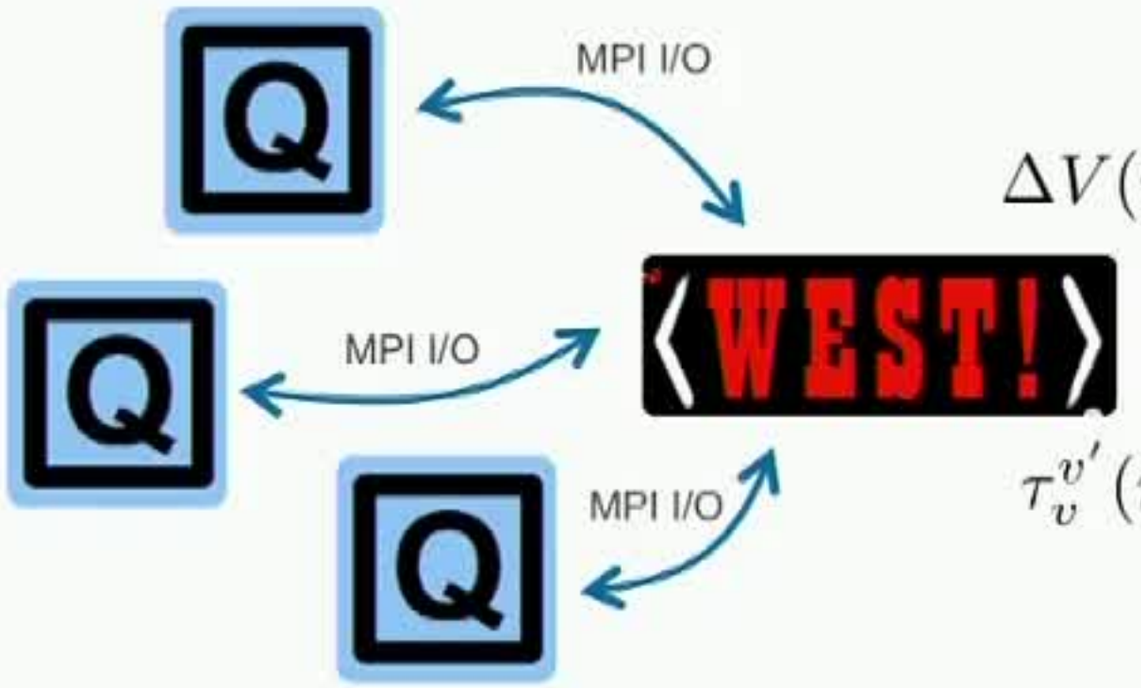
Finite field calculations to solve the Bethe Salpeter equation

$$K^{\mathrm{1d}}_{v,v'}|a_{v'}\rangle = \hat{\mathbf{P}}_c\Big(\int \mathbf{W}(\mathbf{r},\mathbf{r}')\varphi^{o*}_{v'}(\mathbf{r}')\varphi^{o}_{v}(\mathbf{r}')d\mathbf{r}'\Big)|a_{v'}\rangle$$

$$\hat{\mathbf{W}} = \mathbf{v_c} + \mathbf{v_c}\chi\mathbf{v_c}$$

$$\hat{H} = \hat{H}_o + \Delta V(r)$$

$$\Delta\rho(r) = \sum_v \varphi^{o*}_v(r) \times [\varphi_v(r) - \varphi^o_v(r)]$$



$$\Delta V(r) = \int \mathbf{v_c}(\mathbf{r},\mathbf{r}')\rho^{v'}_v(r')dr'$$

$$\tau^{v'}_v(r) = \int \hat{\mathbf{W}}(\mathbf{r},\mathbf{r}')\varphi^*_{v'}(r)\varphi_v(r)$$

$$= \Delta V + \int v_c(r,r')\Delta\rho(r')dr'$$

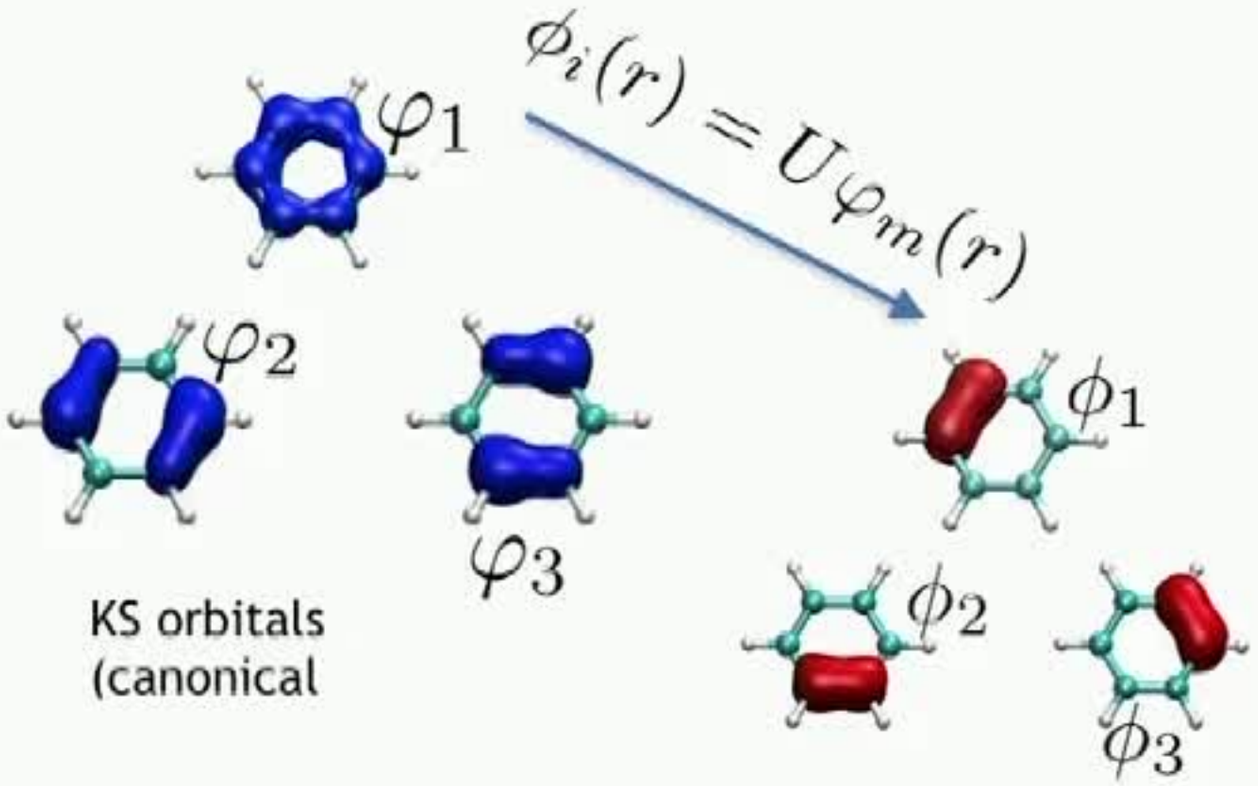
http://qboxcode.org/ http://www.west-code.org/

Nguyen, Govoni, Gygi, Galli (submitted)

Reduction of scaling from N^4 to N^3

$$K^{1\mathrm{d}}_{v,v'}|a_{v'}\rangle = \underset{U^\dagger}{\hat{\mathbf{P}}_c}\Big(\int \underset{U^\dagger}{\mathbf{W}(\mathbf{r},\mathbf{r}')}\underset{U}{\varphi^{o*}_{v'}(\mathbf{r}')}\underset{U}{\varphi^{o}_{v}(\mathbf{r}')}d\mathbf{r}'\Big)|a_{v'}\rangle$$

$$U^\dagger U = I$$

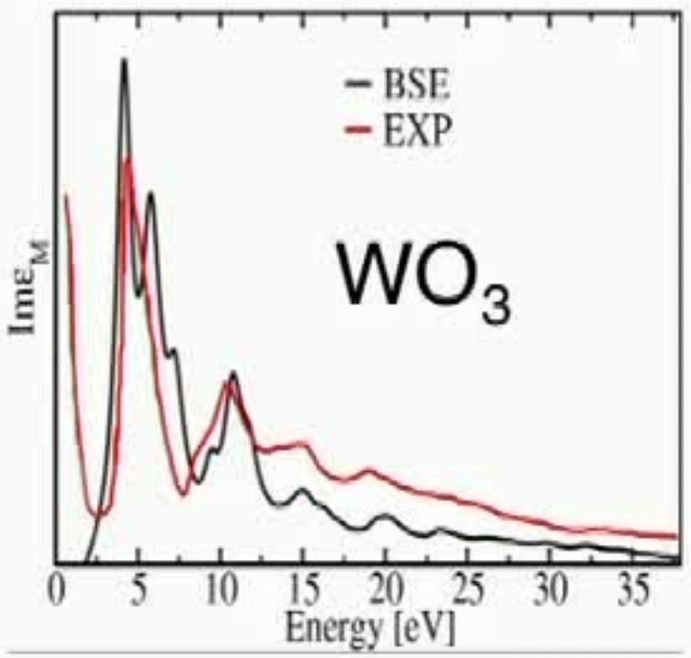


$$\varphi_1(r) \times \varphi_2(r) \neq 0$$

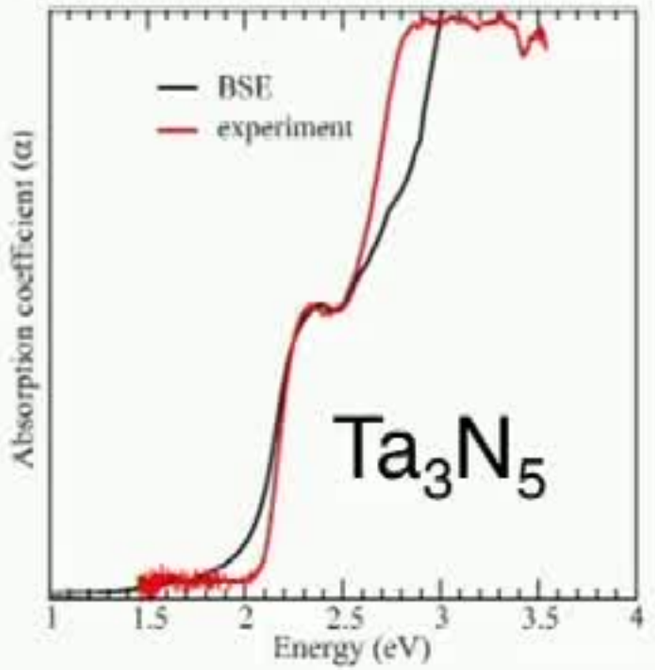
$$\phi_1(r) \times \phi_2(r) \sim 0$$

Some examples

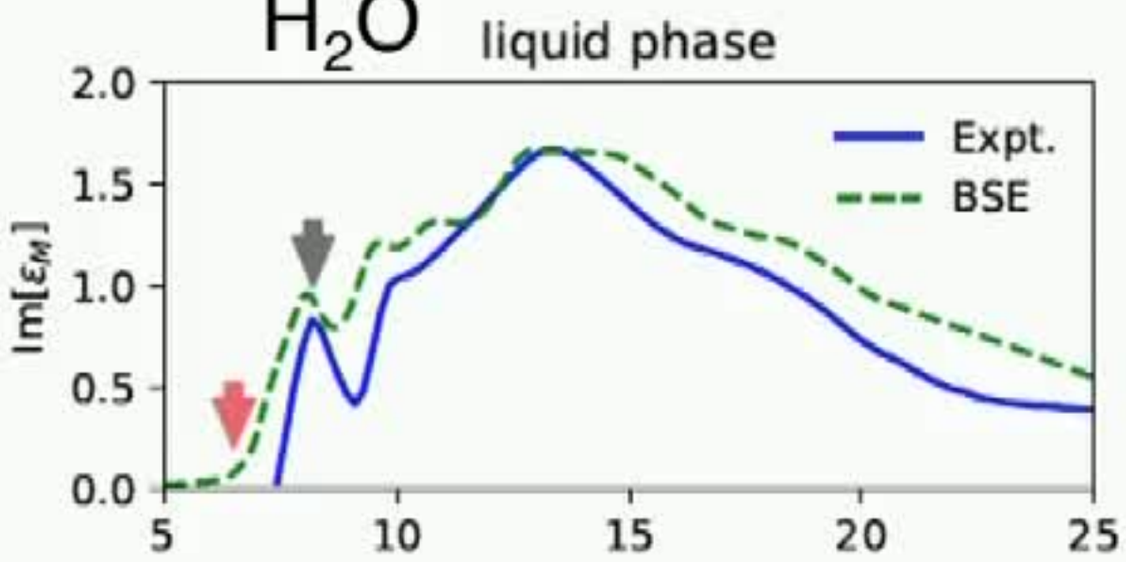
Absorption spectra: solids & liquids

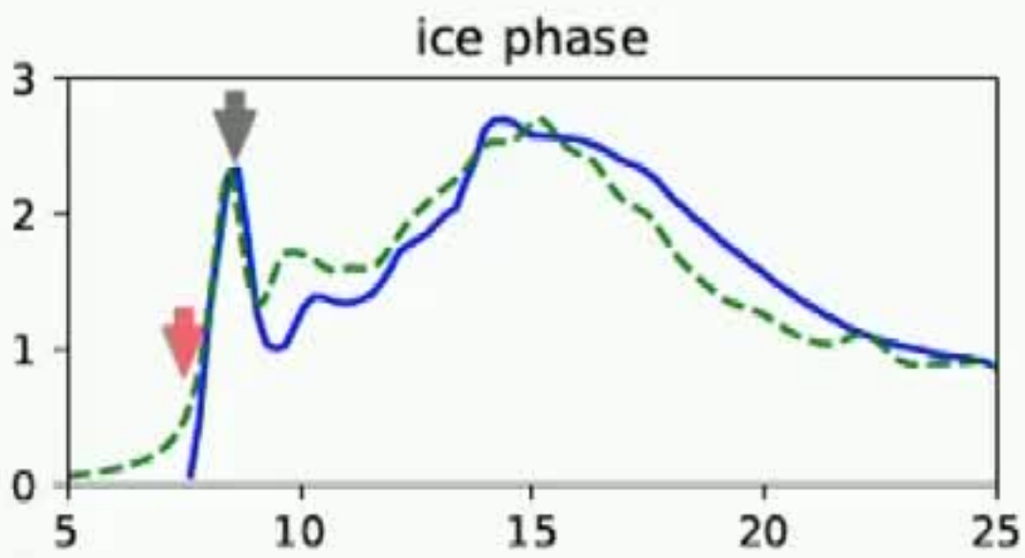


PRB 2013;



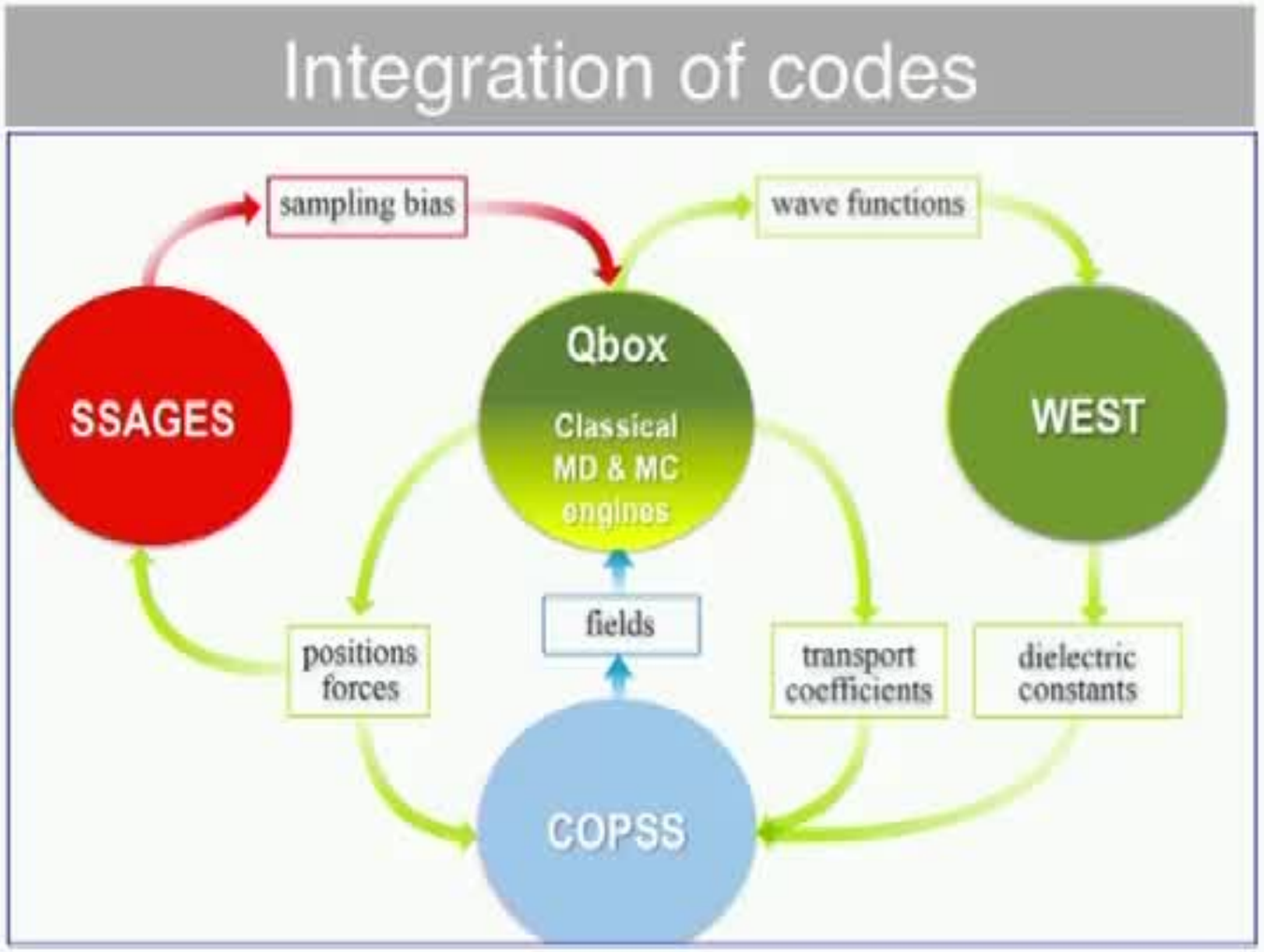
PRB 2014 & 2016





Method developments & software interoperability

- **WEST**
  - —Many-body perturb. theory
    http://www.west-code.org
- **Qbox**
  - —First-principles MD
    http://qboxcode.org
- **SSAGES**
  - —Advanced sampling
    http://miccomcodes.org/
- **COPSS**
  - — Particle-continuum codes
    http://miccomcodes.org/

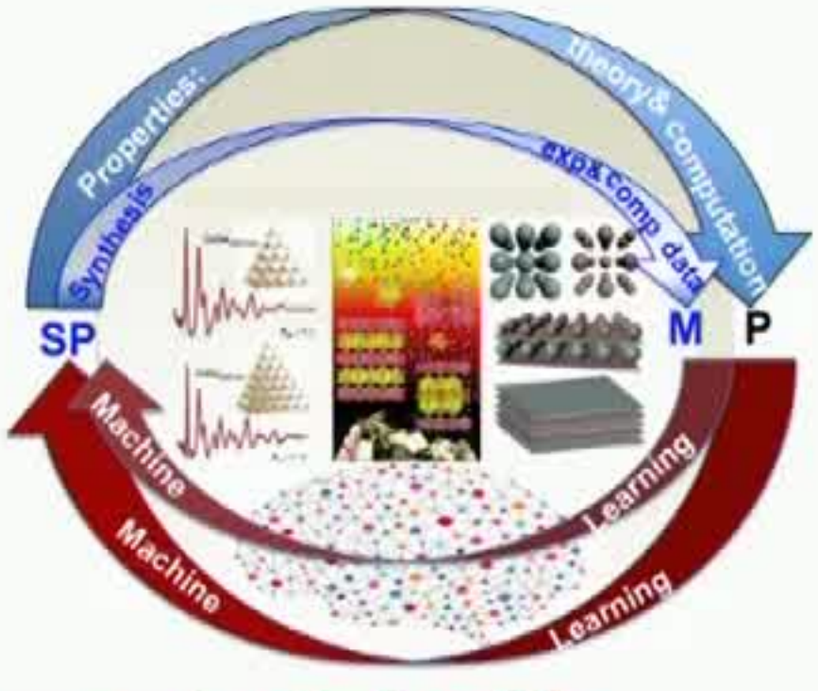


http://miccom-center.org/software.html

MICCoM

Discovery & Design

- 'Inverse problems' : not yet there
  —The road to progress will include the ability to carry out *robust & efficient* calculations of *many* materials *properties*



- Predictions on how to synthetize a material with desired properties: not yet there
  —Computational synthesis requires brand new theoretical and computational strategies

- Discovery of new physical phenomena

Towards D&D

Towards D&D

- Coupling of methods & coupling of software
    - Method development (theory & algorithms) is a critical need of the field

- Definition of automatic verification and validation procedures

- Integrated [theory-computation-data-experimental] strategies & automatic feedbacks

Acknowledgements

Qbox:
First-principles molecular dynamics

WEST:
Many-body perturbation theory

SSAGES:
Reactive pathway identification and free energy calculation

NSF

U.S. DEPARTMENT OF ENERGY

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http://miccom-center.org

Collaborators: Dmitri Talapin (UoC), Stefan Wipperman (Max Planck, Dusseldorf), Francois Gygi (UCD), Juan de Pablo (UoC), David Awschalom (UoC), Francesco Paesani (UCD), T. Anh Pham (LLNL)