U.S. DOE SciDAC Partnership

Predictive Computing for Condensed Matter

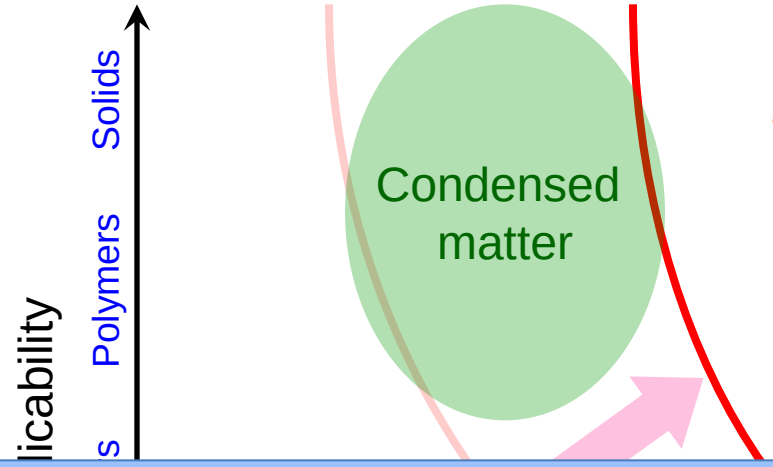
Garnet Chan (Chemistry)
Bryan Clark (Physics)

So Hirata (Chemistry)
Peter Abbamonte (Physics)
David Ceperley (Physics)
Shinsei Ryu (Physics)
Lucas Wagner (Physics)

Shiwei Zhang (Physics)

UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

Frontiers of predictive computing



Size consistency
Finite temperature, finite pressure
Metals, superconductors
Strong correlation
Computational costs

A DOE report on Computational Materials Science (2010):
*"We are at the threshold of a new era where the integrated synthesis, characterization, and **modeling of complex materials** and chemical processes **will transform our ability to understand and design new materials and chemistries** with predictive power"*

Materials Genome Initiative for Global Competitiveness (2011):
*"the development of advanced materials can be accelerated through advances in **computational techniques**"*

The team

So Hirata (Chemistry, UIUC) - Lead PI

Hirata is a theoretical/computational chemist and an expert in electron-correlation theories for molecules and solids. He is the primary author of the computer-generated, high-rank electron-correlation modules in DOE's massively parallel NWCHEM suite of software, implemeting several of his original methods.

Lucas Wagner (Physics, UIUC) - Co-lead PI

Wagner is the principal author of the quantum Monte Carlo program, QWALK, with which he has performed predictively accurate calculations on strongly correlated systems.

Peter Abbamonte (Physics, UIUC)

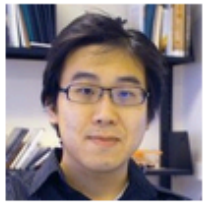
Abbamonte, an experimental condensed-matter physicist, brings an invaluable experimental insight into the project. He is one of the originators of resonant soft x-ray scattering, with which he discovered a Wigner crystal in doped spin ladders and the charged stripes in copper-oxide superconductors.

David Ceperley (Physics & NCSA, UIUC)

Ceperley is a theoretical/computational physicist and an authority of quantum Monte Carlo (QMC). He invented a number of QMC algorithms and is the author of massively parallel QMCPACK software.

Garnet K.-L. Chan (Chemistry, Princeton)

Chan is a recognized expert in strong correlation theories including density matrix renormalization group (DMRG), tensor networks, and density matrix functional theory. He has, in particular, established DMRG as a practical, powerful tool for strongly correlated molecular electronic structures.



Bryan Clark (Microsoft Station Q)

Clark has considerable experience in both conventional quantum Monte Carlo (QMC) and novel extensions such as QMC in the Hilbert space. He has developed a large-scale parallel algorithm of QMC in PIMC++.

Shinsei Ryu (Physics, UIUC)

Ryu specializes in mathematical theories of strong correlation and other condensed phase electronic structures. Ryu is a pioneer in the use of entanglement entropy in classifying topological phases of matter and has predicted the fractional topological insulator in two dimension.

Shiwei Zhang (Physics, W&M)

Zhang specializes in computational condensed matter physics and materials science. Zhang is a pioneer in the use of quantum Monte Carlo (QMC) in the Hilbert space for strong correlation. He is the inventor of the phaseless auxiliary field QMC.

Project goals

Theories

(Finite-*T*) MP, CC, RPA, etc.; QMC; DMRG, TN; FCIQMC, AFQMC, MC-MP2; DMFT

Software

Algorithm redesign; massive parallelism; fast integrals

Applications – experimental verification

Metals; (copper oxide) superconductors; graphene; molecular crystals; Peierls systems and Luttinger liquid; Mott-Hubbard systems; spin liquid

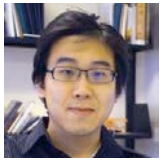
Abbamonte

Theories

Hirata

Finite-temperature
MP2, CCD, RPA

Monte Carlo MP2



Chan

Clark

Wave function theory

Zhang

AFQMC

DMRG

DMFT

FCIQMC

Ceperley

Quantum Monte Carlo

Strong correlation

Wagner

Ryu

DMC, VMC

TN (MERA, PEPS)

Schrödinger equation
for water

10-particle, 30-dimensional partial differential equation

$$\overbrace{\left(-\frac{\hbar^2}{2m_e}\sum_{i=1}^{10}\nabla_i^2-\frac{\hbar^2}{2m_I}\sum_{I=1}^{3}\nabla_I^2-\sum_{I=1}^{3}\sum_{i=1}^{10}\frac{Z_I e^2}{4\pi\varepsilon_0 r_{iI}}+\sum_{i=1}^{9}\sum_{j=i+1}^{10}\frac{e^2}{4\pi\varepsilon_0 r_{ij}}+\sum_{I=1}^{2}\sum_{J=I+1}^{3}\frac{Z_I Z_J e^2}{4\pi\varepsilon_0 r_{IJ}}\right)}^{\hat{H}}\Psi=E\Psi$$

$$\frac{\partial^2}{\partial r_i^2}+\frac{2}{r_i}\frac{\partial}{\partial r_i}+\frac{1}{r_i^2}\left(\frac{1}{\sin^2\theta_i}\frac{\partial^2}{\partial\phi_i^2}+\frac{1}{\sin\theta_i}\frac{\partial}{\partial\theta_i^2}\sin\theta_i\frac{\partial}{\partial\theta_i^2}\right)$$

Singularities

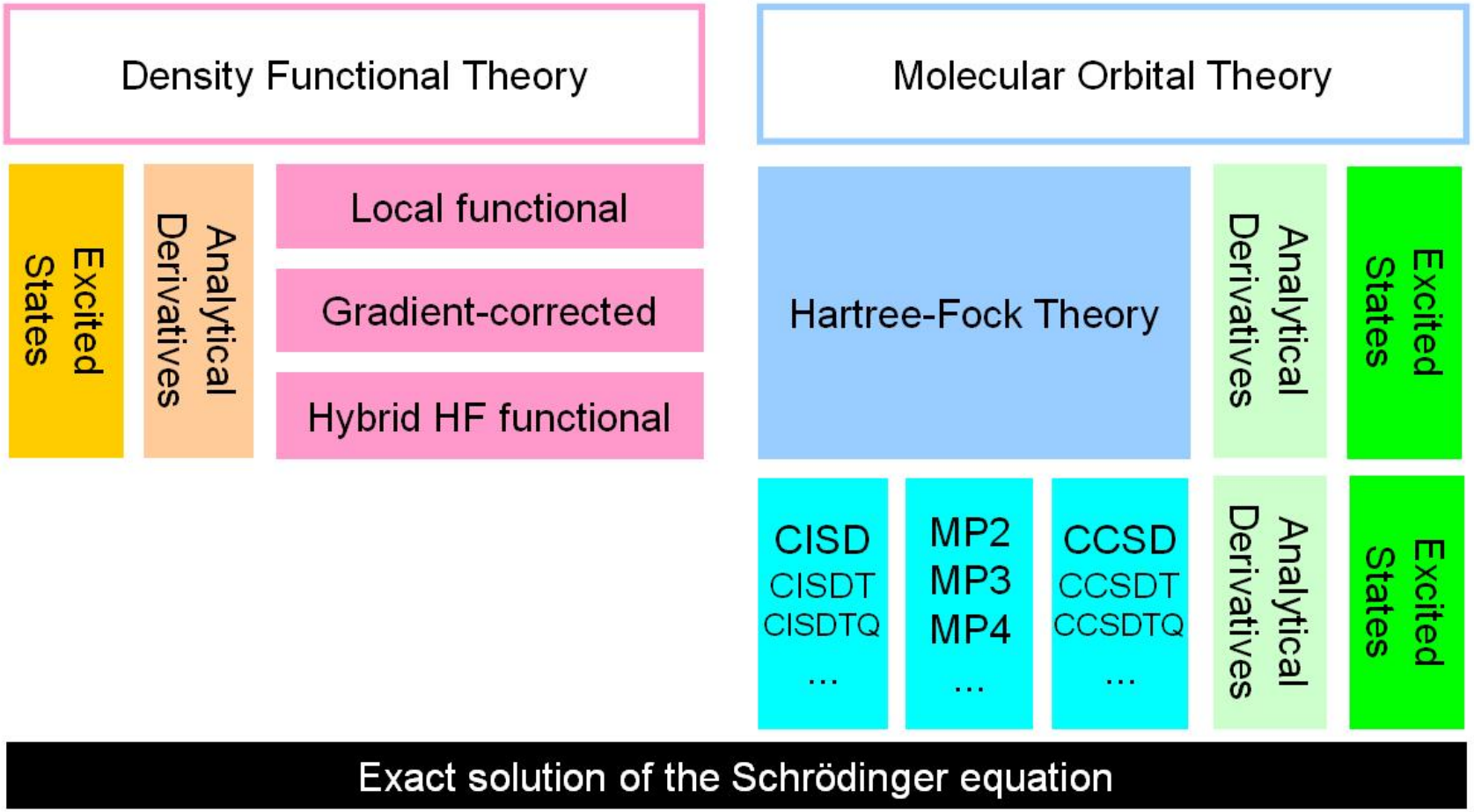
Conditions arising from the indistinguishability of electrons

$$\Psi(\mathbf{r}_{e1},\mathbf{r}_{e2},\mathbf{r}_{e3},\mathbf{r}_{e4},\mathbf{r}_{e5},\mathbf{r}_{e6},\mathbf{r}_{e7},\mathbf{r}_{e8},\mathbf{r}_{e9},\mathbf{r}_{e10},\mathbf{r}_{H1},\mathbf{r}_{H2},\mathbf{r}_O)=$$
$$-\Psi(\mathbf{r}_{e2},\mathbf{r}_{e1},\mathbf{r}_{e3},\mathbf{r}_{e4},\mathbf{r}_{e5},\mathbf{r}_{e6},\mathbf{r}_{e7},\mathbf{r}_{e8},\mathbf{r}_{e9},\mathbf{r}_{e10},\mathbf{r}_{H1},\mathbf{r}_{H2},\mathbf{r}_O)=$$
$$\Psi(\mathbf{r}_{e3},\mathbf{r}_{e1},\mathbf{r}_{e2},\mathbf{r}_{e4},\mathbf{r}_{e5},\mathbf{r}_{e6},\mathbf{r}_{e7},\mathbf{r}_{e8},\mathbf{r}_{e9},\mathbf{r}_{e10},\mathbf{r}_{H1},\mathbf{r}_{H2},\mathbf{r}_O)=$$
$$-\Psi(\mathbf{r}_{e3},\mathbf{r}_{e2},\mathbf{r}_{e1},\mathbf{r}_{e4},\mathbf{r}_{e5},\mathbf{r}_{e6},\mathbf{r}_{e7},\mathbf{r}_{e8},\mathbf{r}_{e9},\mathbf{r}_{e10},\mathbf{r}_{H1},\mathbf{r}_{H2},\mathbf{r}_O)=\ldots$$

Many-body

3,628,800 terms!

Systematic many-body methods



MP2

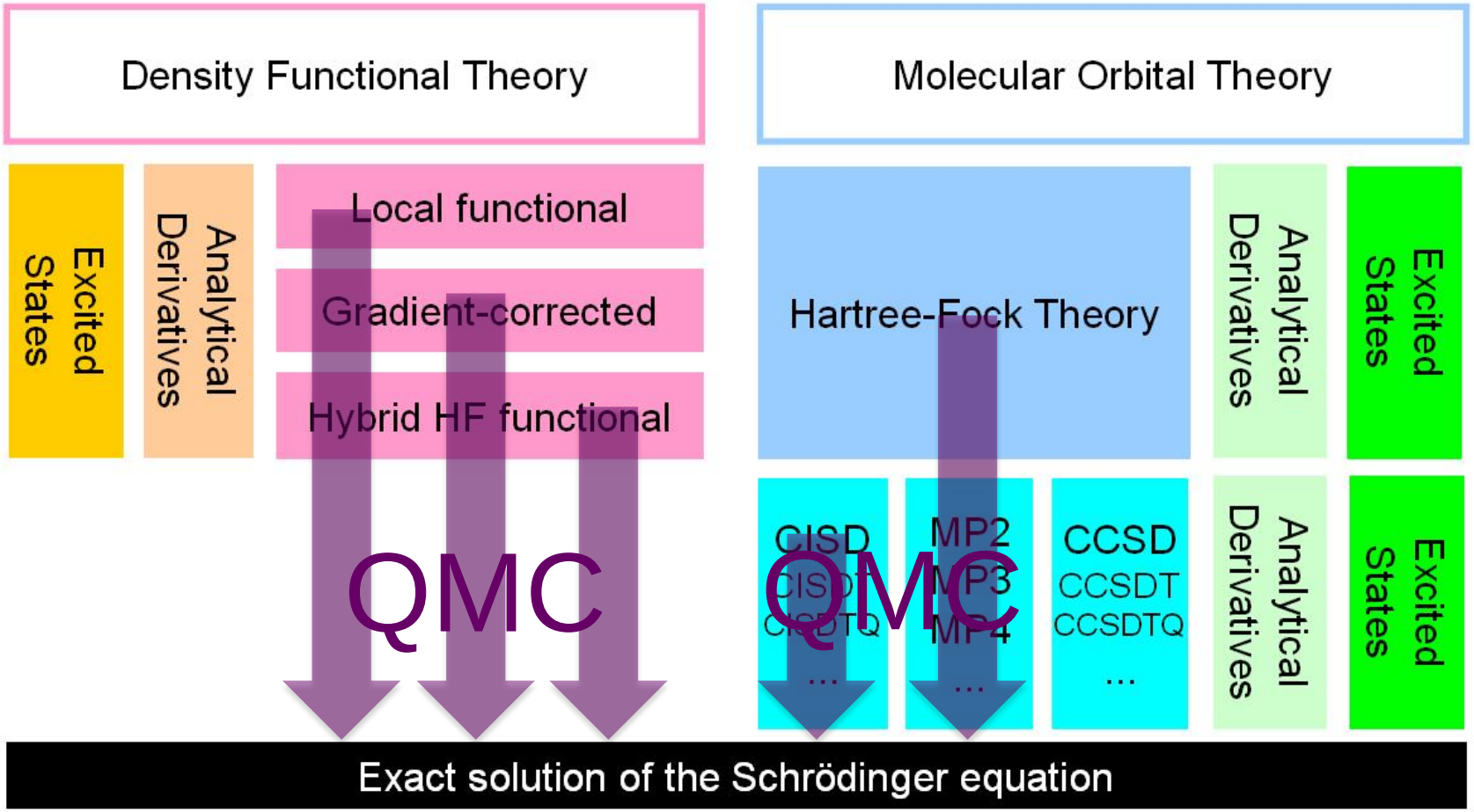
$$\langle ij|ab\rangle = \int \frac{\varphi_i^*(\mathbf{r}_1)\varphi_j^*(\mathbf{r}_2)\varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2)}{|\mathbf{r}_1-\mathbf{r}_2|} d\mathbf{r}_1\, d\mathbf{r}_2$$

- A member of a systematic series of approximations converging toward exactness.
- Can describe covalent, ionic, hydrogen-bond, and dispersion interactions.
- Size consistent and thus applicable to solids.
- Accurate energy bands and band gaps.
- The operation cost grows as $O(n^5)$, where n is the number of orbitals.
- The memory cost grows as $O(n^2)$ to $O(n^4)$.
- Parallelization is difficult.

Laplace-transform MP2 *Canonical MP2*

$$E^{(2)} = -\frac{1}{4}\sum_{i,j}^{\text{occ.}}\sum_{a,b}^{\text{virt.}}\langle ij|ab\rangle\langle ab|ij\rangle\int_0^\infty e^{(\varepsilon_i+\varepsilon_j-\varepsilon_a-\varepsilon_b)\tau}\,d\tau = \frac{1}{4}\sum_{i,j}^{\text{occ.}}\sum_{a,b}^{\text{virt.}}\frac{\langle ij|ab\rangle\langle ab|ij\rangle}{\varepsilon_i+\varepsilon_j-\varepsilon_a-\varepsilon_b}$$

Systematic many-body methods

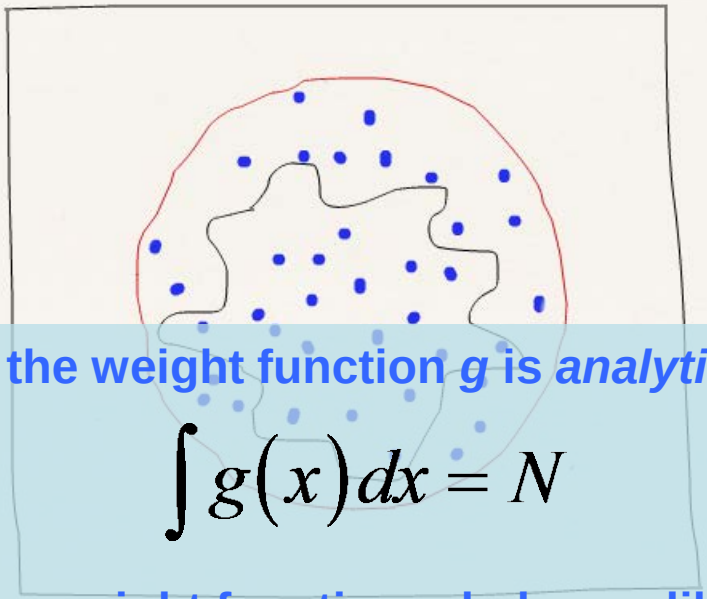


Monte Carlo

$$E = \int f(x)dx = \int \frac{f(x)}{g(x)} g(x)dx = \frac{1}{N}\int \frac{f(x)}{g(x)} g(x)dx \approx \sum_{x \in g} \frac{f(x)}{g(x)} \cdot \int g(x)dx$$

weight function

Metropolis



Requirement 1: **the weight function *g* is *analytically* integrable**

$$\int g(x)dx = N$$

Requirement 2: **the weight function *g* behaves like the integrand *f***

$$f(x)/g(x)$$

Quantum Monte Carlo

$$\hat{H}\Psi = E\Psi$$

$$E = \int \Psi^* \hat{H} \Psi \, d\mathbf{r} \Big/ \int \Psi^* \Psi \, d\mathbf{r}$$

- Gives the *best* wave function and energy in the variational sense, which is usually nearly exact.
- Easily and efficiently parallelized.
- Nearly zero memory cost.
- Has statistical errors, which decay slowly as $O(N^{-1/2})$ with the number of MC steps (N).
- Calculations of structures and properties (including energy bands) and applications to excited states difficult.

$$\hat{H}\Psi / \Psi = E$$

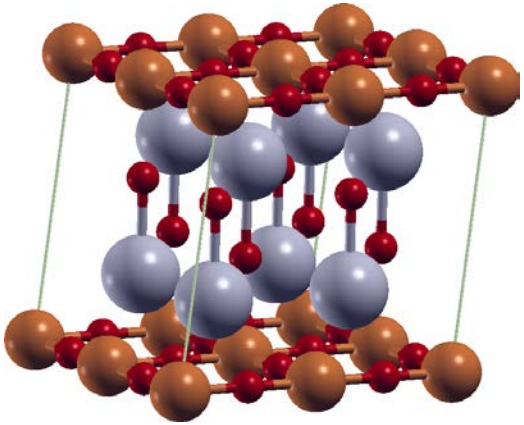
Contents

- Research highlights of 2012-2013
  - QMC for copper oxide superconductors
  - Auxiliary field QMC for band gaps
  - Full CI QMC for excited states
- Monte Carlo MP2 and MP3
- MP2 for molecular crystals: solid-solid phase transition in CO_2

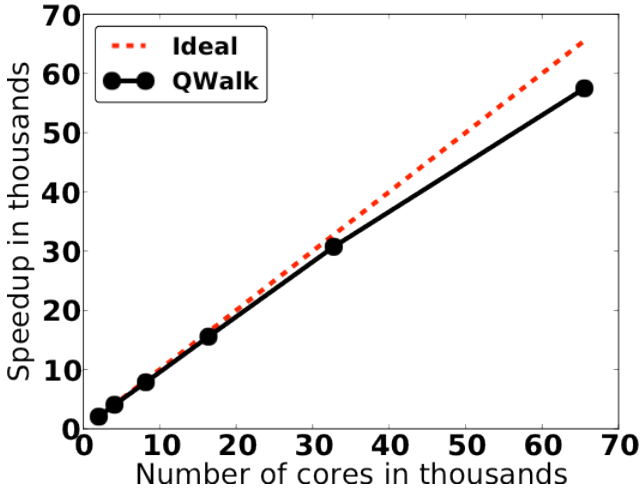
QMC for copper oxide superconductors

Wagner and Abbamonte, to be published (2013)

Wagner



La_2CuO_4

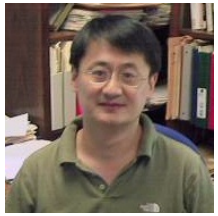


Method	*J* / eV	Magnetic moment
DFT (LDA)	0.82	0.3
DFT (GGA)	0.6	0.5
QMC	**0.15**	**0.62**
Expt	**0.13**	**0.6**

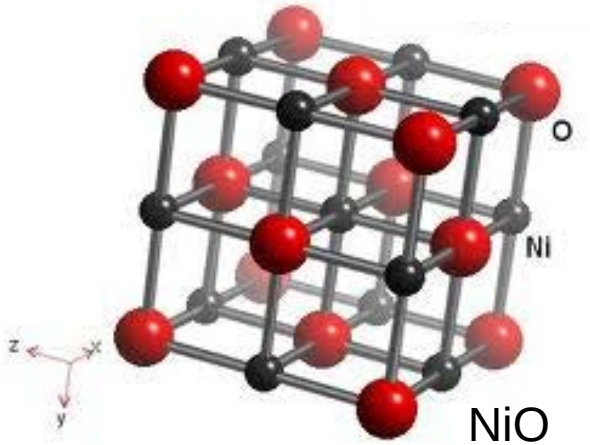
For more details, please visit the poster by Lucas Wagner

Auxiliary field QMC for band gaps

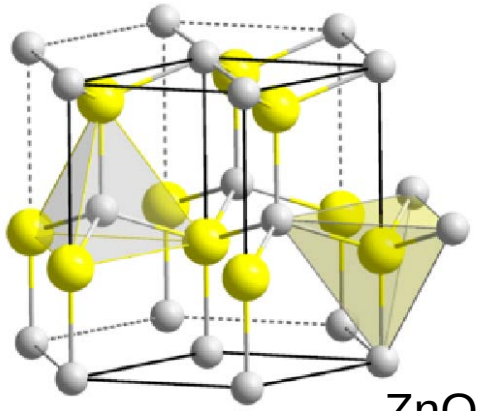
Zhang *et al.*, to be published (2013)



Zhang



NiO



ZnO

Method	Band gap / eV
DFT (LDA)	0.67
GW	4.8
QMC	**3.97**
Expt	**3.7, 3.87, 4.0, 4.3**

Method	Band gap / eV
DFT (LDA)	1.0
GW	2.4, 2.6, 2.8
QMC	**3.26**
Expt	**3.3 – 3.57**

Full CI QMC for excited states

Booth and Chan, *JCP Comm* (2012)

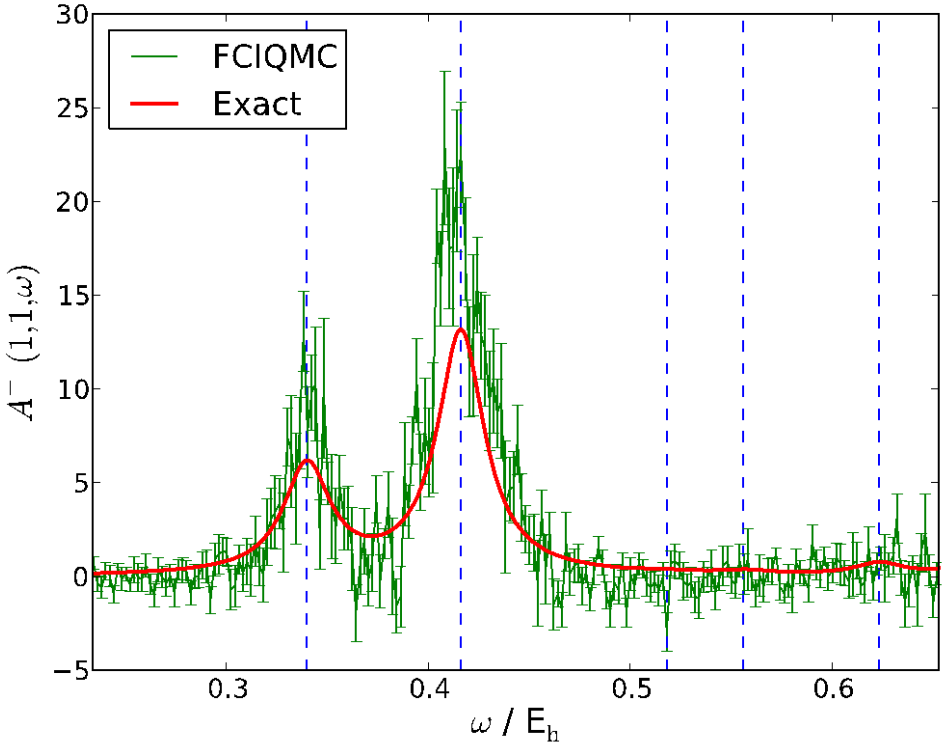
Chan

$$\exp[-\beta(H-E)]$$

Standard propagator:
max at ground-state

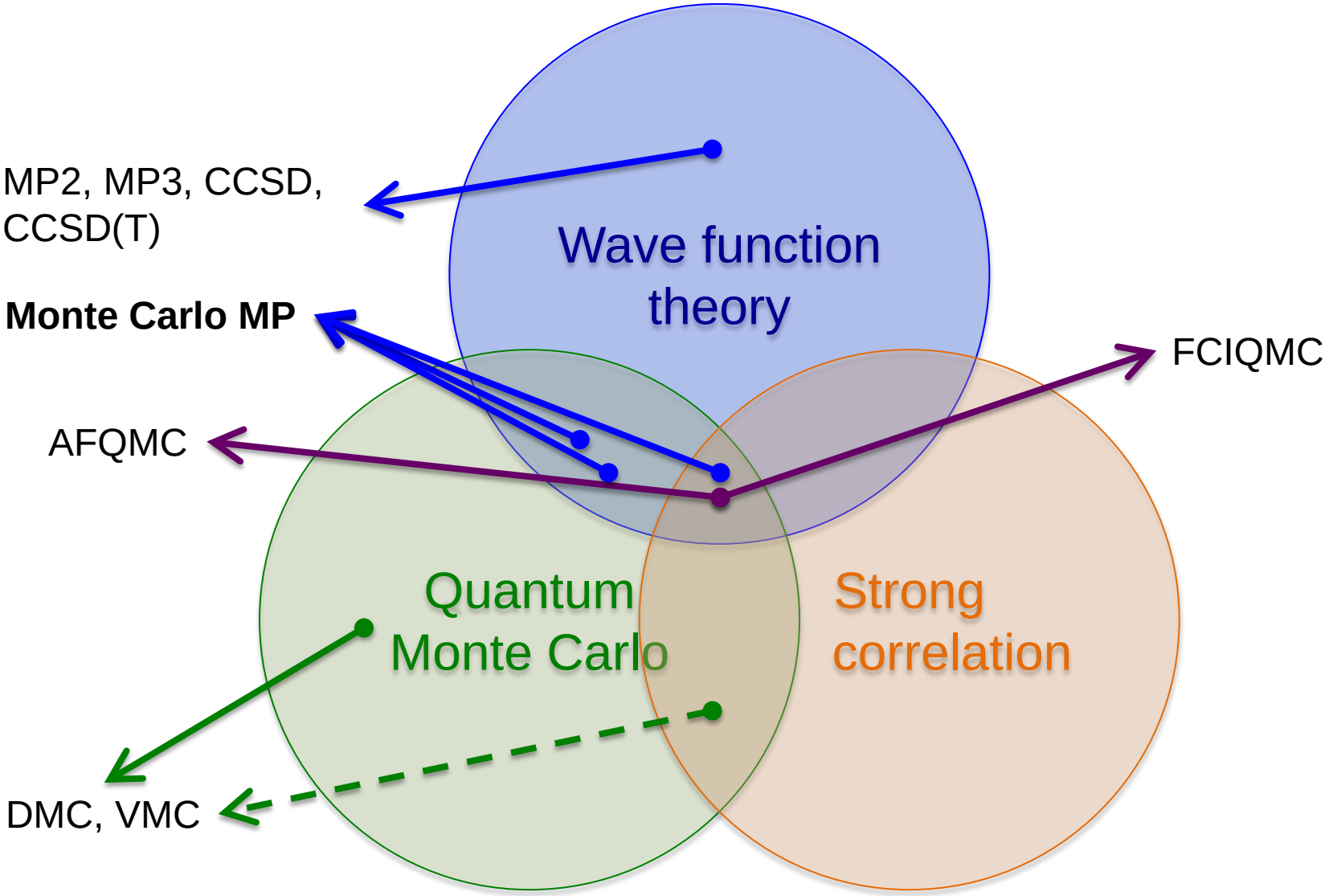
$$\exp[-\beta(H-\omega)^2]$$

Gaussian propagator:
max at specified omega



Monte Carlo MP

Willow, Kim and Hirata, *JCP* (2012), *JCP* (2013), under review by *JCTC* (2013)



Monte Carlo MP2

Willow, Kim and Hirata, *JCP* (2012)

Very long $O(n^4)$ summation of products of 2 x 6-dimensional integrals

$$E^{(2)} = \sum_{i,j}^{\text{occ.}} \sum_{a,b}^{\text{vir.}} \frac{\langle ab|ij\rangle\langle ij|ab\rangle}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

Explicit two-electron integrals

$$E^{(2)} = \sum_{i,j}^{\text{occ.}} \sum_{a,b}^{\text{vir.}} \frac{\int \varphi_i(\mathbf{r}_1)\varphi_j(\mathbf{r}_2)\frac{1}{r_{12}}\varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2 \int \varphi_i(\mathbf{r}_3)\varphi_j(\mathbf{r}_4)\frac{1}{r_{34}}\varphi_a(\mathbf{r}_3)\varphi_b(\mathbf{r}_4)d\mathbf{r}_3 d\mathbf{r}_4}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

Laplace transformation of the denominator

$$E^{(2)} = -\sum_{i,j}^{\text{occ.}} \sum_{a,b}^{\text{vir.}} \int \varphi_i(\mathbf{r}_1)\varphi_j(\mathbf{r}_2)\frac{1}{r_{12}}\varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2 \int \varphi_i(\mathbf{r}_3)\varphi_j(\mathbf{r}_4)\frac{1}{r_{34}}\varphi_a(\mathbf{r}_3)\varphi_b(\mathbf{r}_4)d\mathbf{r}_3 d\mathbf{r}_4 \int_0^\infty e^{(\varepsilon_i+\varepsilon_j-\varepsilon_a-\varepsilon_b)\tau} d\tau$$

Change of orders of summations and integrations

$$E^{(2)} = -\int\cdots\int\int_0^\infty \frac{\sum_i^{\text{occ.}} \varphi_i(\mathbf{r}_1)\varphi_i(\mathbf{r}_3)e^{\varepsilon_i\tau} \sum_j^{\text{occ.}} \varphi_j(\mathbf{r}_2)\varphi_j(\mathbf{r}_4)e^{\varepsilon_j\tau} \sum_a^{\text{vir.}} \varphi_a(\mathbf{r}_1)\varphi_a(\mathbf{r}_3)e^{-\varepsilon_a\tau} \sum_b^{\text{vir.}} \varphi_b(\mathbf{r}_2)\varphi_b(\mathbf{r}_4)e^{-\varepsilon_b\tau}}{r_{12}r_{34}} d\mathbf{r}_1\cdots d\mathbf{r}_4\, d\tau$$

Single 13-dimensional integral evaluated by Monte Carlo

$$E^{(2)} = -\int\cdots\int\int_0^\infty \frac{G^-(\mathbf{r}_1,\mathbf{r}_3,\tau)G^-(\mathbf{r}_2,\mathbf{r}_4,\tau)G^+(\mathbf{r}_1,\mathbf{r}_3,\tau)G^+(\mathbf{r}_2,\mathbf{r}_4,\tau)}{r_{12}r_{34}} d\mathbf{r}_1\cdots d\mathbf{r}_4\, d\tau$$

Monte Carlo MP2

Willow, Kim and Hirata, *JCP* (2012)

$$E = \int f(x)dx = \int \frac{f(x)}{g(x)} g(x)dx = \sum_{x \in g} \frac{f(x)}{g(x)} \cdot \int g(x)dx$$

weight function

Metropolis

Requirement 1: **analytically integrable** $\int g(x)dx = N$

Requirement 2: **cancellation of singularities** $f(x)/g(x)$

$$E^{(2)} = -\int \cdots \int \int_0^\infty \frac{G^-(\mathbf{r}_1,\mathbf{r}_3,\tau)G^-(\mathbf{r}_2,\mathbf{r}_4,\tau)G^+(\mathbf{r}_1,\mathbf{r}_3,\tau)G^+(\mathbf{r}_2,\mathbf{r}_4,\tau)}{r_{12}\, r_{34}} d\mathbf{r}_1 \cdots d\mathbf{r}_4\, d\tau$$

Singularities

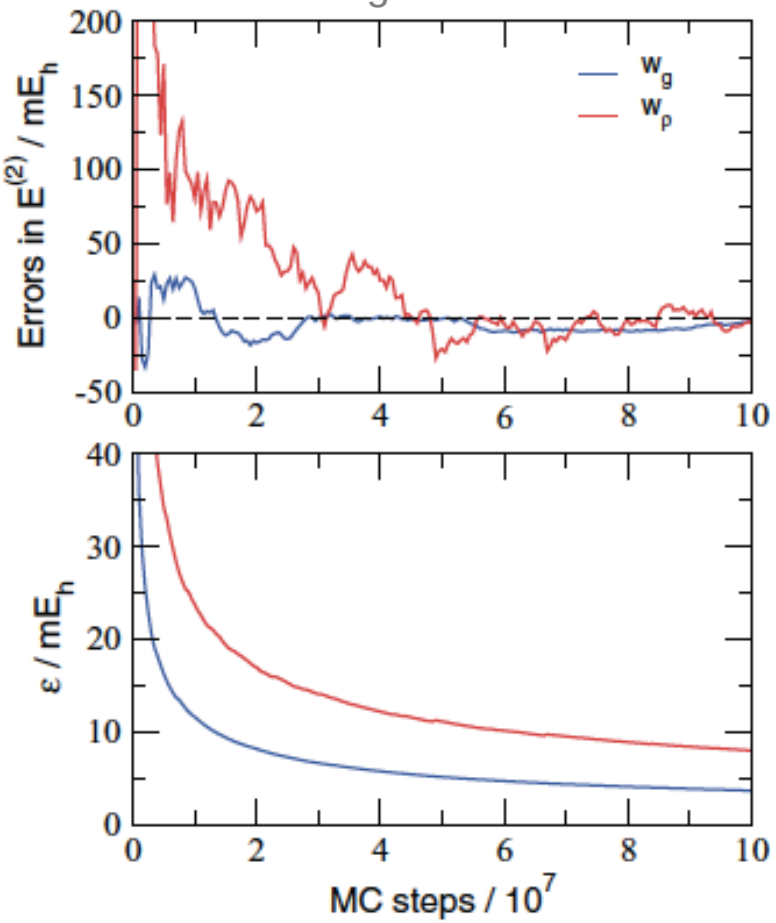
$$g(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4) = \frac{\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)}{r_{12}} \frac{\rho(\mathbf{r}_3)\rho(\mathbf{r}_4)}{r_{34}}$$

$$\int g(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4) d\mathbf{r}_1\, d\mathbf{r}_2\, d\mathbf{r}_3\, d\mathbf{r}_4 = 4E^2_{\text{Coulomb}}$$

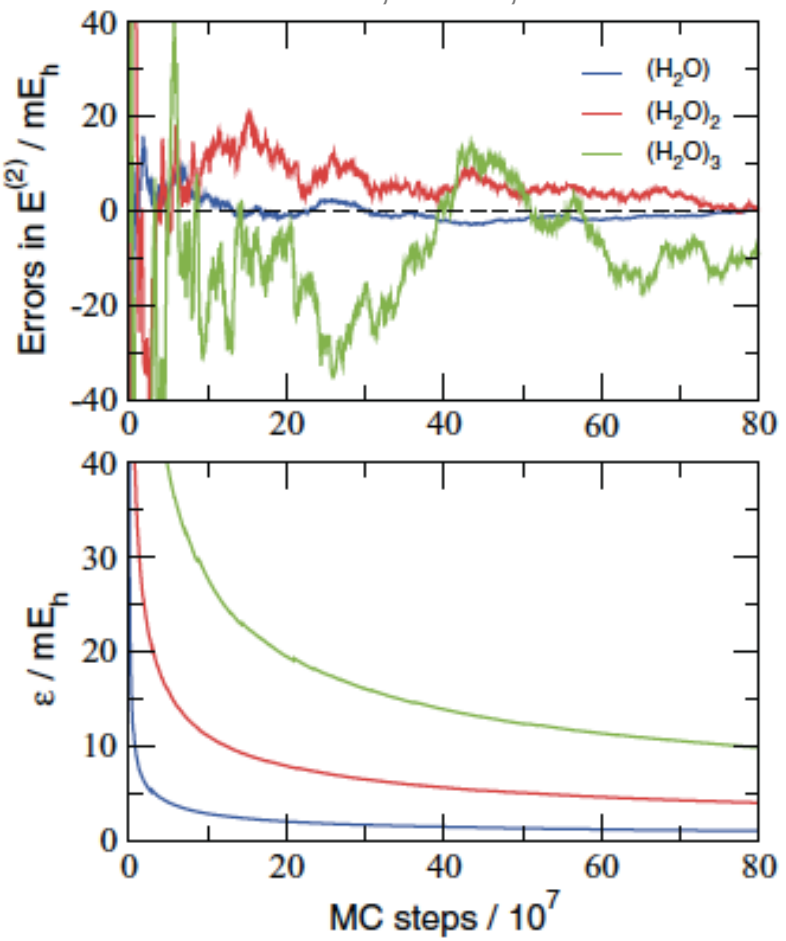
Monte Carlo MP2

Willow, Kim and Hirata, *JCP* (2012)

Nitrogen 6-31G**



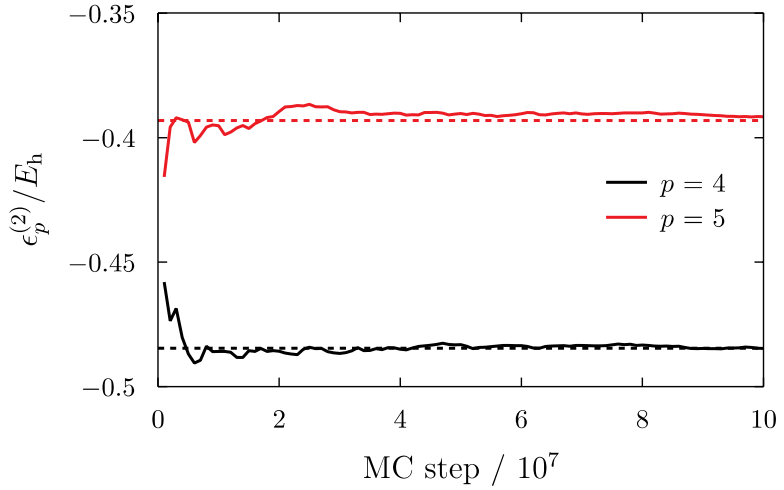
Water monomer, dimer, trimer 6-31G**



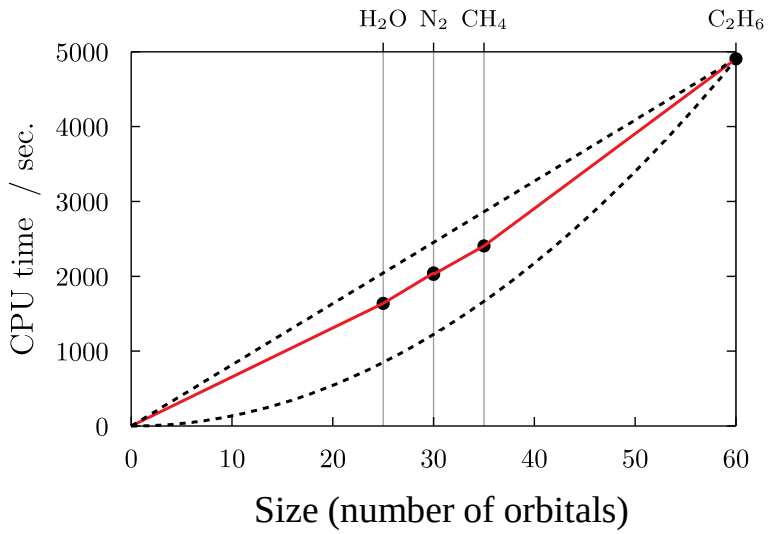
Monte Carlo MP2 for self-energies

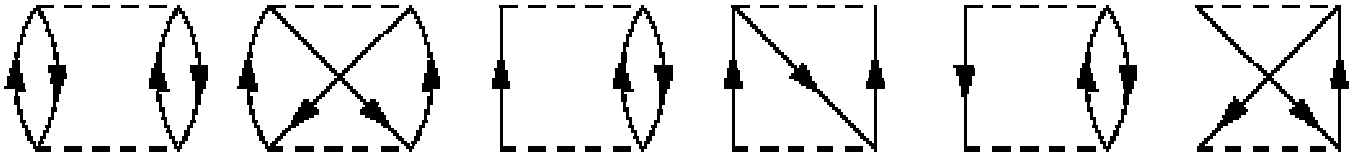
Willow, Kim and Hirata, *JCP* (2013)

HOMO & HOMO−1 of H_2O



Efficiency

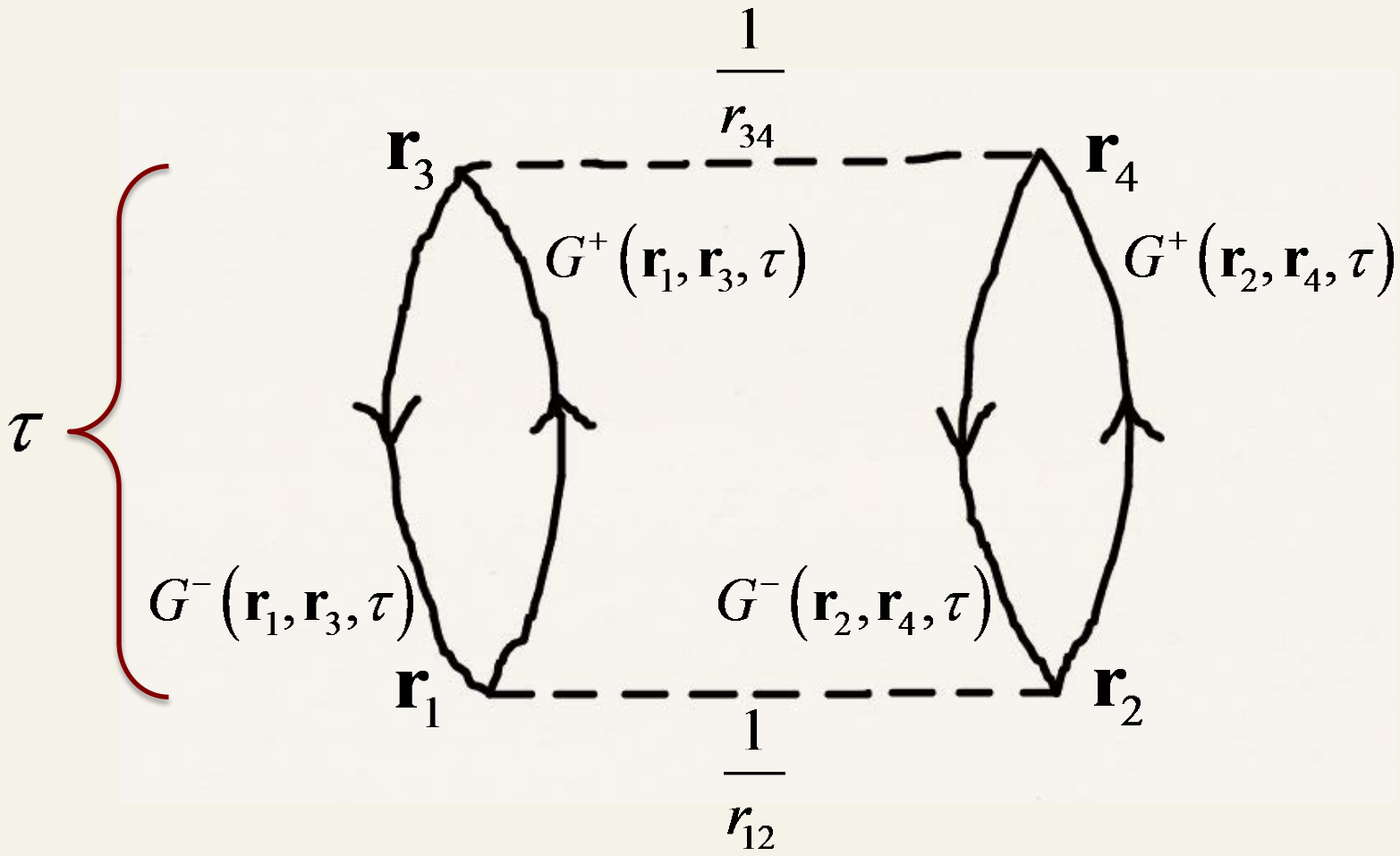




Dyson self-energies (quasiparticle energies) for multiple states obtainable from a single MC run

Real-space Green's function

Willow, Kim and Hirata, to be published (2013)

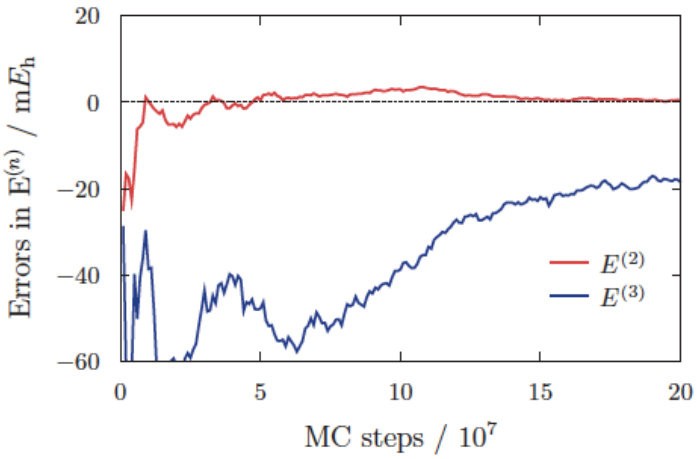


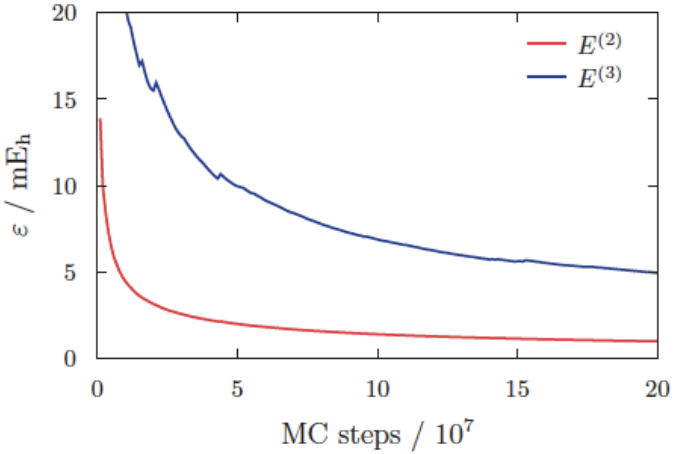
$$E^{(2)} = -\int\cdots\int\int_0^\infty \frac{G^-(\mathbf{r}_1,\mathbf{r}_3,\tau)G^-(\mathbf{r}_2,\mathbf{r}_4,\tau)G^+(\mathbf{r}_1,\mathbf{r}_3,\tau)G^+(\mathbf{r}_2,\mathbf{r}_4,\tau)}{r_{12}r_{34}} d\mathbf{r}_1\cdots d\mathbf{r}_4\, d\tau$$

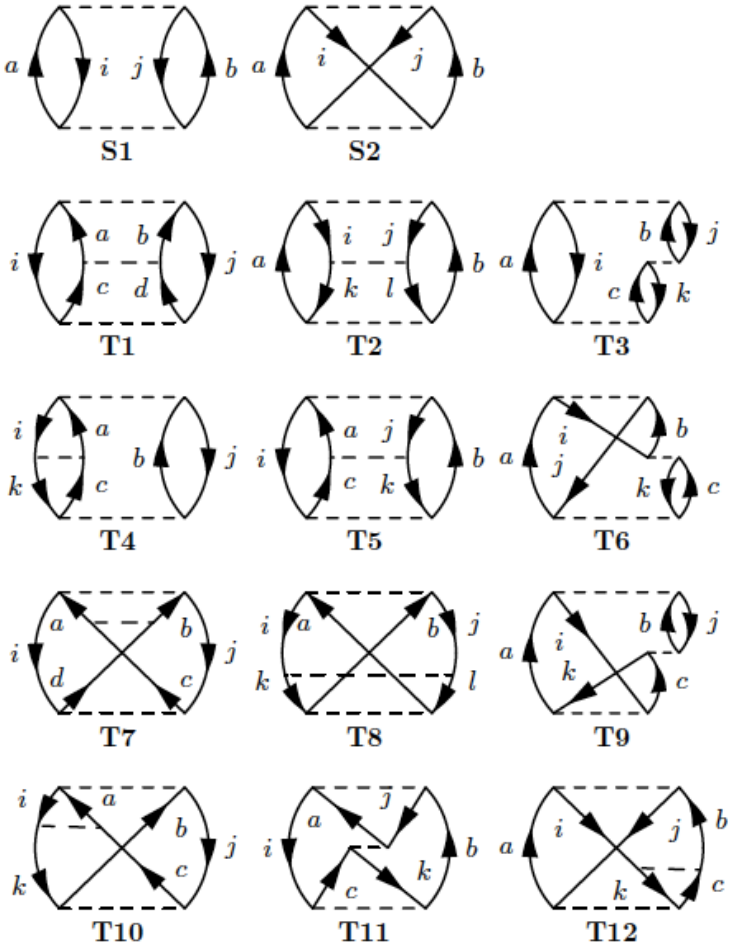
Monte Carlo MP3

Willow, Kim and Hirata, to be published (2013)

Water 6-31G**



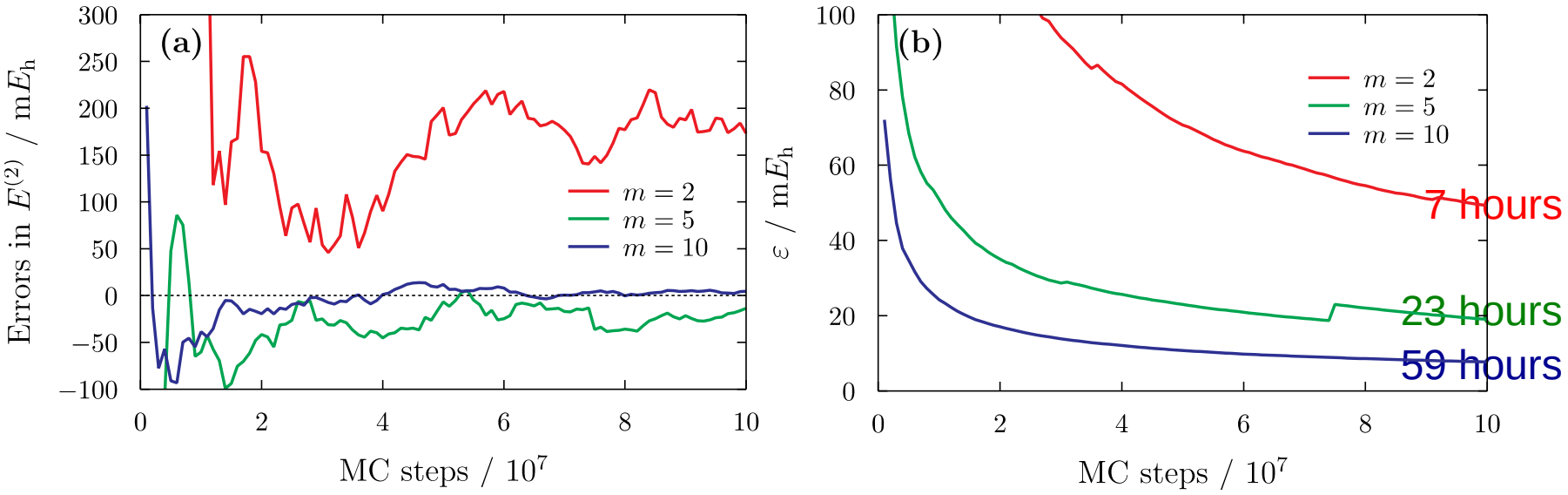




Redundant-walker MC-MP2

Willow, Hermes, Kim and Hirata, under review by *JCTC* (2013)

Benzene 6-31G**



m = 2: 2 electron walker pairs

$$E^{(2)} = -\int\int\int_0^\infty \frac{G^-(\mathbf{r}_1,\mathbf{r}_3,\tau)G^-(\mathbf{r}_2,\mathbf{r}_4,\tau)G^+(\mathbf{r}_1,\mathbf{r}_3,\tau)G^+(\mathbf{r}_2,\mathbf{r}_4,\tau)}{r_{12}r_{34}} d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 d\mathbf{r}_4 d\tau$$

m = 10: 10 electron walker pairs

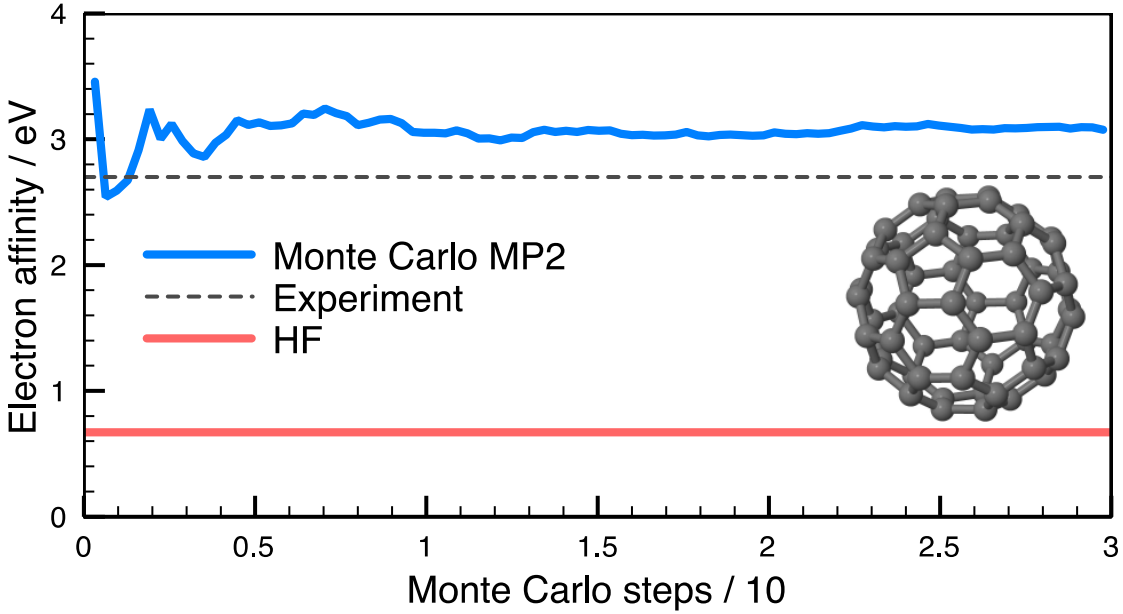
Cost: **5 times**

Benefit: 10 x 9 / 2 = **45 times** MC steps

Massively parallel MC-MP2

Willow, Hermes, Kim and Hirata, under review by *JCTC* (2013)

C_{60} cc-pVDZ on 320 processors of Blue Waters

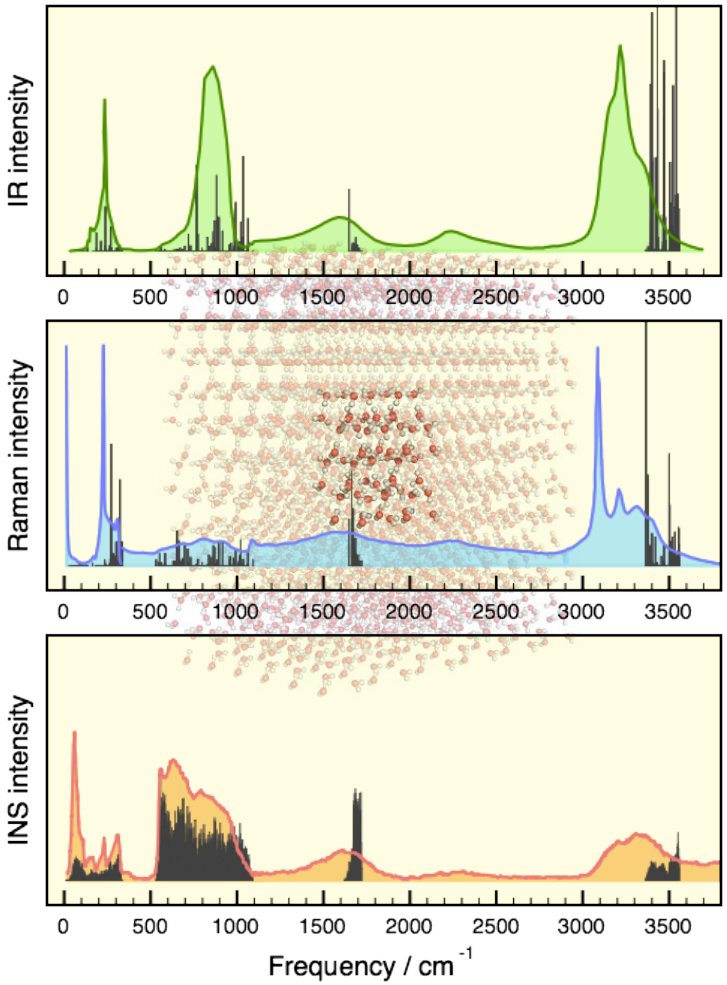


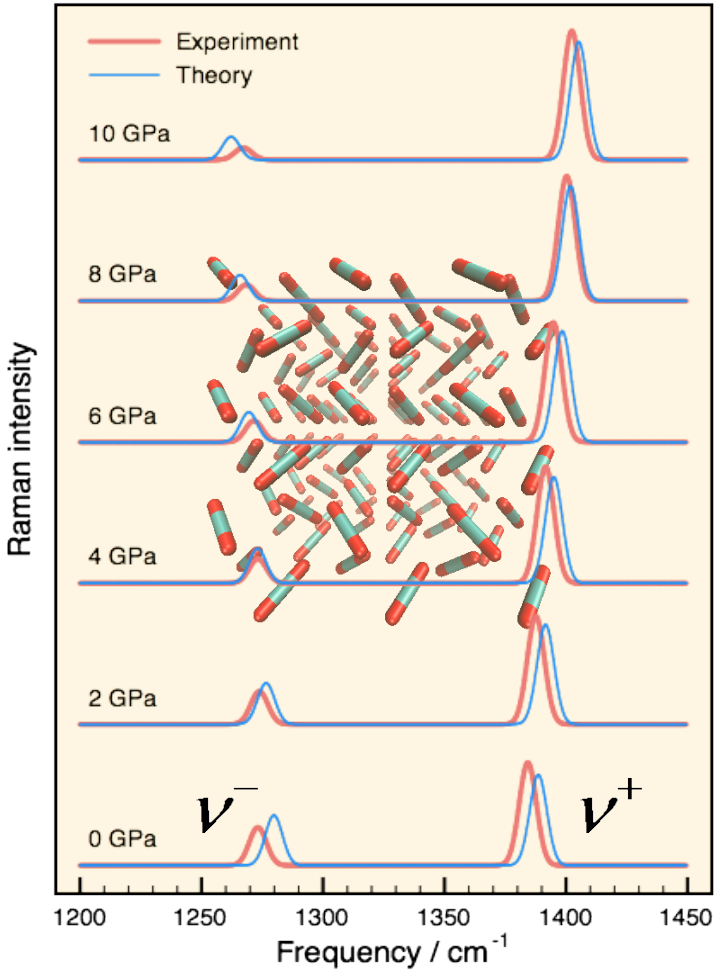
m = 120: 120 electron walker pairs

Cost: **60 times**

Benefit: 120 x 119 / 2 = **7140 times** MC steps

MP2 for molecular crystals



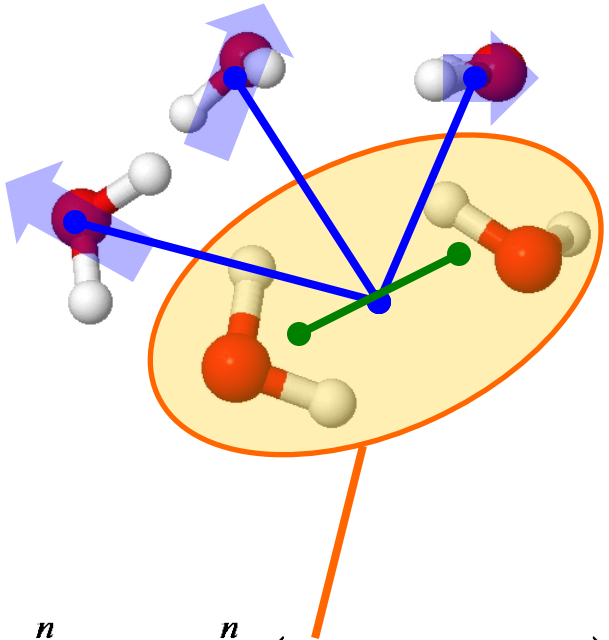


Embedded-fragment approach

Hirata *et al*., *MP* (2005); Kamiya, Hirata, and Valiev, *JCP* (2008)

***N*-body (*N* > 2) Coulomb in point-charge or dipole approximation**

1 and 2-body
Coulomb
Exchange
Correlation



Pair energy in the presence of self-consistent atomic charges or dipoles

$$E = \sum_{i=1}^{n} E'_i + \sum_{i<j}^{n} \left(E'_{ij} - E'_i - E'_j \right) + \square$$

Molecular crystals

Hirata, *JCP* (2008)

Energy per unit cell

$$E = \sum_i E_{i(0)} + \sum_{i<j} \left\{ E_{i(0)\,j(0)} - E_{i(0)} - E_{j(0)} \right\} + \frac{1}{2} \sum_{m=-L}^{+L} (1-\delta_{m0}) \sum_{i,j} \left\{ E_{i(0)\,j(m)} - E_{i(0)} - E_{j(m)} \right\}$$

Energy gradients

$$\frac{\partial E}{\partial x} \approx \sum_i \frac{\partial E_{i(0)}}{\partial x} + \sum_{i<j} \left\{ \frac{\partial E_{i(0)\,j(0)}}{\partial x} - \frac{\partial E_{i(0)}}{\partial x} - \frac{\partial E_{j(0)}}{\partial x} \right\} + \frac{1}{2} \sum_{m=-L}^{+L} (1-\delta_{m0}) \sum_{i,j} \left\{ \frac{\partial E_{i(0)\,j(m)}}{\partial x} - \frac{\partial E_{i(0)}}{\partial x} - \frac{\partial E_{j(m)}}{\partial x} \right\}$$

$$\frac{\partial E}{\partial a} \approx \frac{1}{2} \sum_{m=-L}^{+L} \sum_{i,j} \sum_{\gamma} m \left\{ \frac{\partial E_{i(0)\,j(m)}}{\partial z_\gamma^{j(m)}} - \frac{\partial E_{j(m)}}{\partial z_\gamma^{j(m)}} \right\} + \frac{\partial E_{\mathrm{LR}}}{\partial a}$$

Linear scaling regardless of gradients algorithms (analytical vs. numerical)
Long-range electrostatic correction essential for cell gradients

Energy Hessian

$$\frac{\partial^2 E}{\partial x \partial y} \approx \sum_i \frac{\partial^2 E_{i(0)}}{\partial x \partial y} + \sum_{i<j} \left\{ \frac{\partial^2 E_{i(0)\,j(0)}}{\partial x \partial y} - \frac{\partial^2 E_{i(0)}}{\partial x \partial y} - \frac{\partial^2 E_{j(0)}}{\partial x \partial y} \right\} + \frac{1}{2} \sum_{m=-L}^{+L} (1-\delta_{m0}) \sum_{i,j} \left\{ \frac{\partial^2 E_{i(0)\,j(m)}}{\partial x \partial y} - \frac{\partial^2 E_{i(0)}}{\partial x \partial y} - \frac{\partial^2 E_{j(m)}}{\partial x \partial y} \right\}$$

x and y need not be in-phase coordinates: phonon dispersions can be obtained

Finite pressures and temperatures

Li, Sode, Voth and Hirata, under review by *Nature Comm* (2013)

Gibbs free energy per unit cell

$$G = E + E_{\mathrm{ZP}} + P(abc) - TS$$

For an orthorhombic unit cell

Partition function

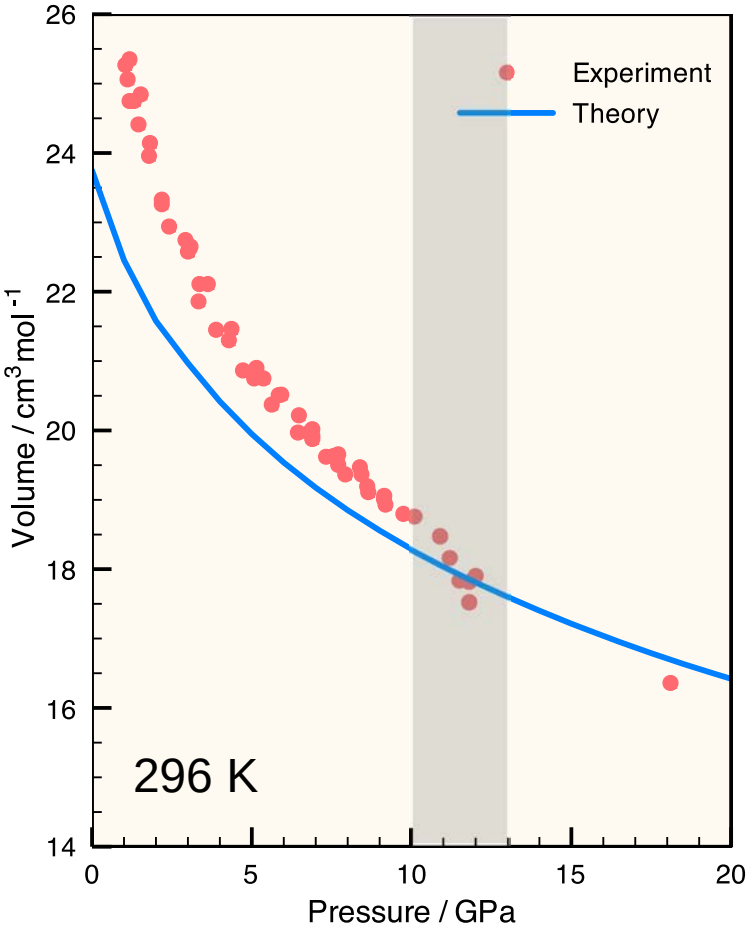
$$Z = \prod_{i} \prod_{\mathbf{k}_i} \frac{\exp\left(-\omega_{i\mathbf{k}_i} / 2k_{\mathrm{B}}T\right)}{1 - \exp\left(-\omega_{i\mathbf{k}_i} / k_{\mathrm{B}}T\right)}$$

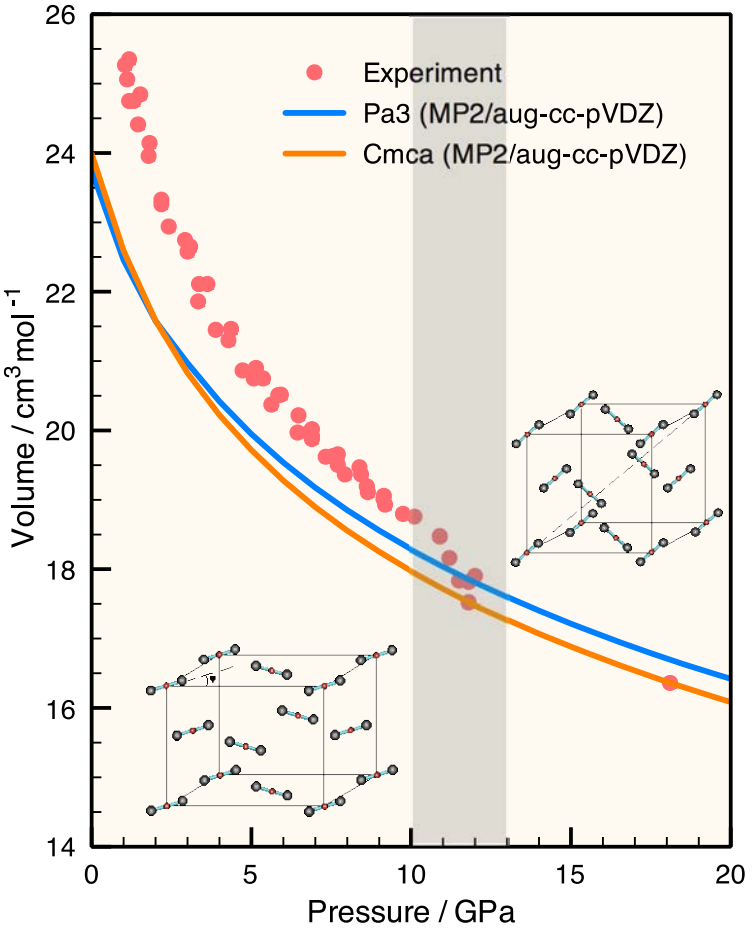
Zero-point energy, entropy, and heat capacity

$$E_{\mathrm{ZP}} = k_{\mathrm{B}}T^2 \frac{\partial \ln Z}{\partial T} \qquad S = -\frac{\partial\left(k_{\mathrm{B}}T \ln Z\right)}{\partial T} \qquad C_{\mathrm{V}} = \frac{\partial\left(E + E_{\mathrm{ZP}}\right)}{\partial T}$$

Phase transition in solid CO_2

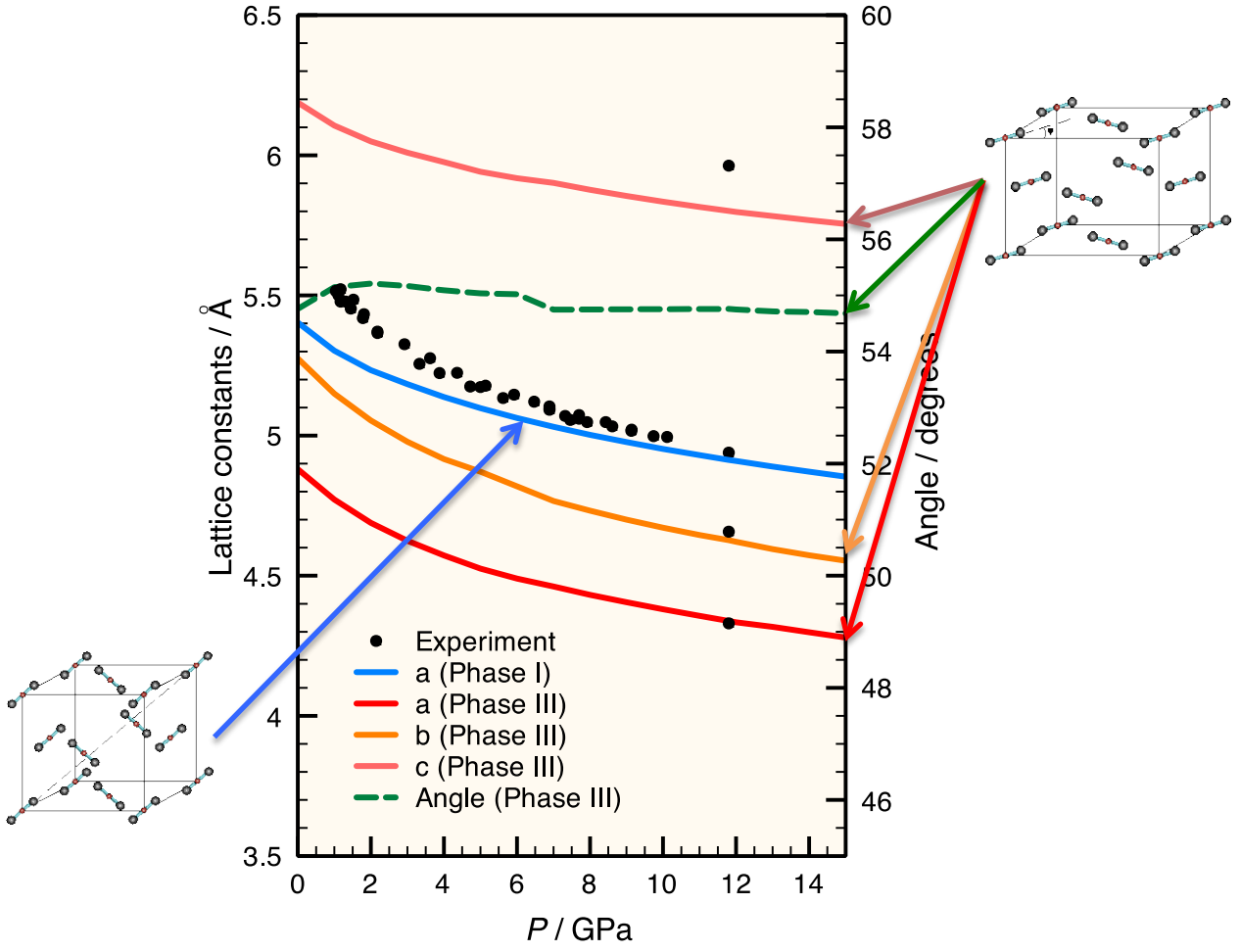
Li, Sode, Voth and Hirata, under review by *Nature Comm* (2013)





Phase transition in solid CO_2

Li, Sode, Voth and Hirata, under review by *Nature Comm* (2013)



Phase transition in solid CO_2

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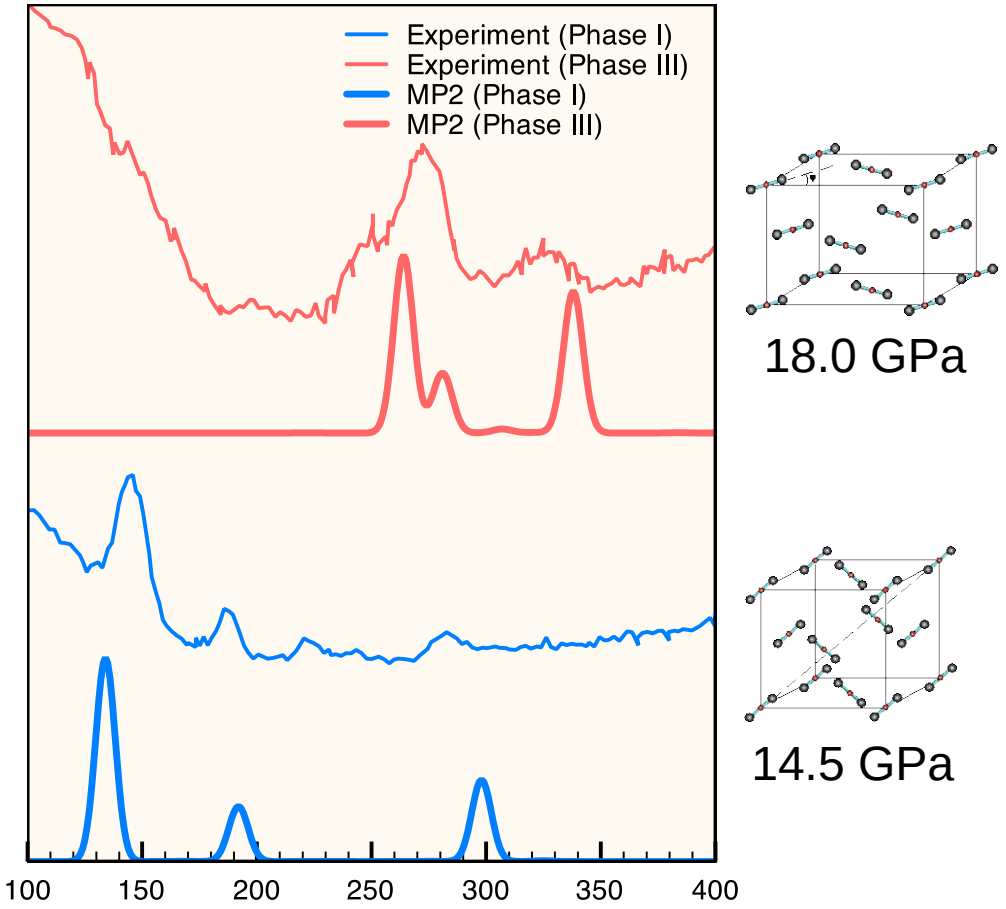

Phase transition in solid CO_2

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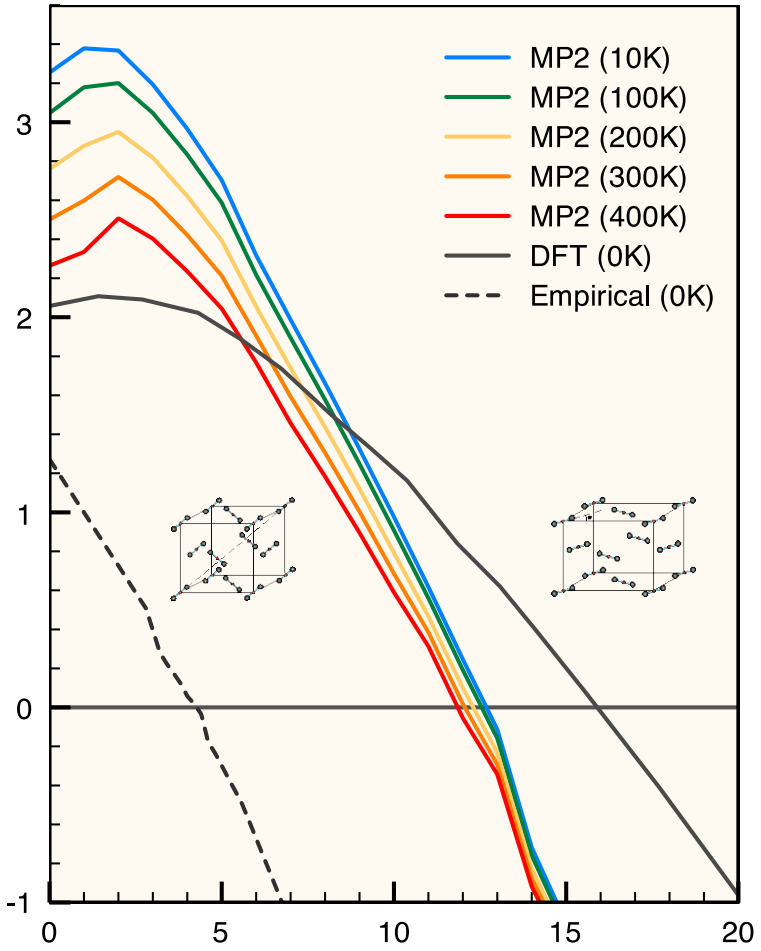

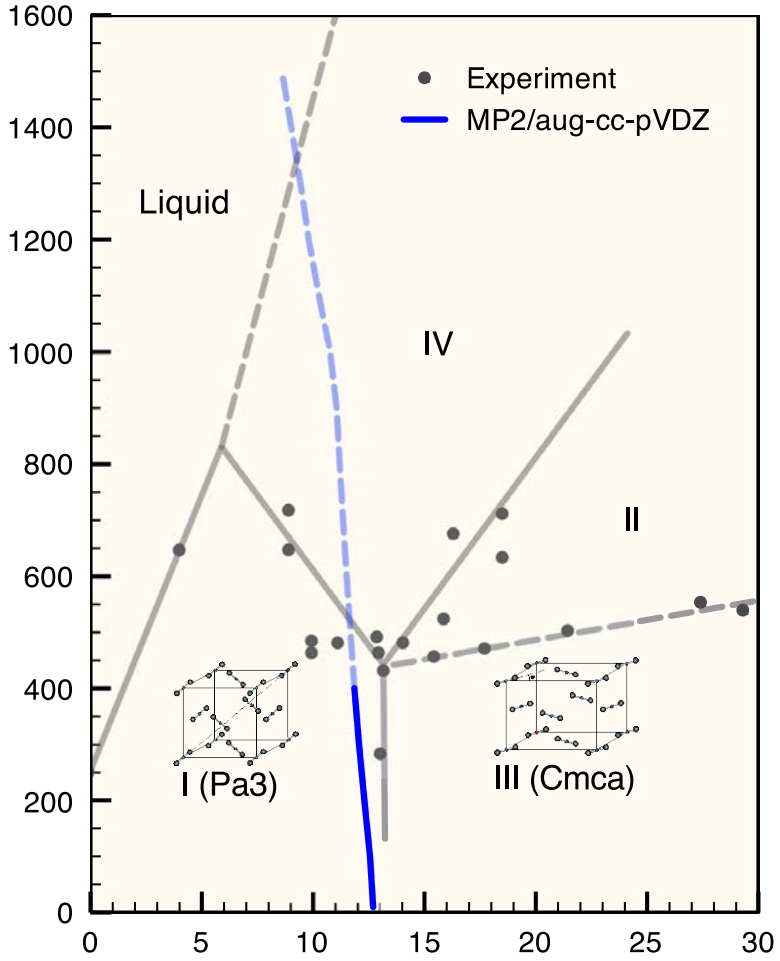

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SciDAC
Scientific Discovery through Advanced Computing

Lucas Wagner (Physics, UIUC) - Co-lead PI

Wagner is the principal author of the quantum Monte Carlo program, QWALK, with which he has performed predictively accurate calculations on strongly correlated systems.

Peter Abbamonte (Physics, UIUC)

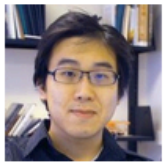
Abbamonte, an experimental condensed-matter physicist, brings an invaluable experimental insight into the project. He is one of the originators of resonant soft x-ray scattering, with which he discovered a Wigner crystal in doped spin ladders and the charged stripes in copper-oxide superconductors.

David Ceperley (Physics & NCSA, UIUC)

Ceperley is a theoretical/computational physicist and an authority of quantum Monte Carlo (QMC). He invented a number of QMC algorithms and is the author of massively parallel QMCPACK software.

Garnet K.-L. Chan (Chemistry, Princeton)

Chan is a recognized expert in strong correlation theories including density matrix renormalization group (DMRG), tensor networks, and density matrix functional theory. He has, in particular, established DMRG as a practical, powerful tool for strongly correlated molecular electronic structures.



Bryan Clark (Microsoft Station Q)

Clark has considerable experience in both conventional quantum Monte Carlo (QMC) and novel extensions such as QMC in the Hilbert space. He has developed a large-scale parallel algorithm of QMC in PIMC++.

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Ryu specializes in mathematical theories of strong correlation and other condensed phase electronic structures. Ryu is a pioneer in the use of entanglement entropy in classifying topological phases of matter and has predicted the fractional topological insulator in two dimension.

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Zhang specializes in computational condensed matter physics and materials science. Zhang is a pioneer in the use of quantum Monte Carlo (QMC) in the Hilbert space for strong correlation. He is the inventor of the phaseless auxiliary field QMC.

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