Predictive Computing for Solids and Liquids

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Schrödinger equation
for a water molecule

10-particle, 30-dimensional partial differential equation

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

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

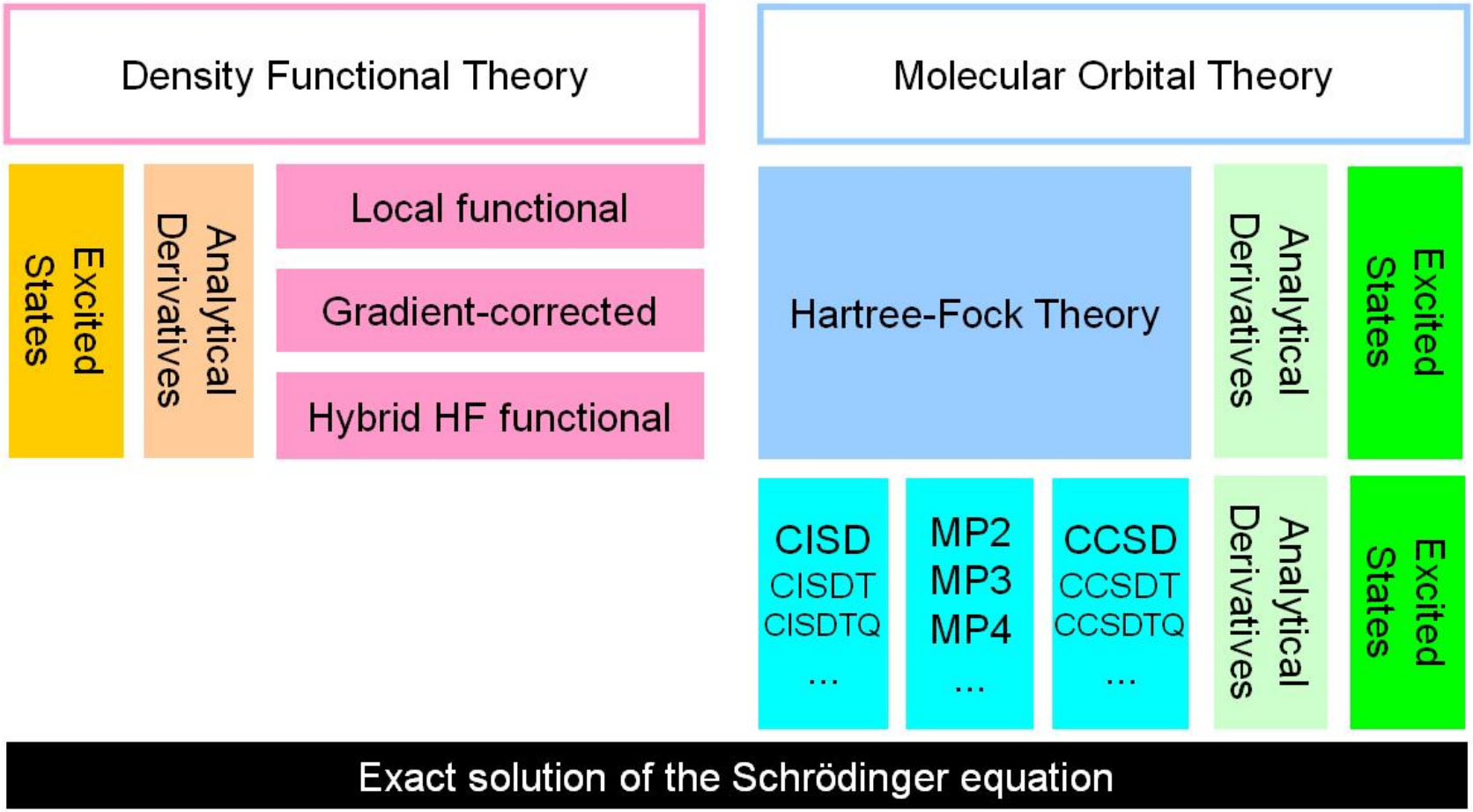
Conditions arising from the indistinguishability of electrons

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

Many-body

3,628,800 terms!

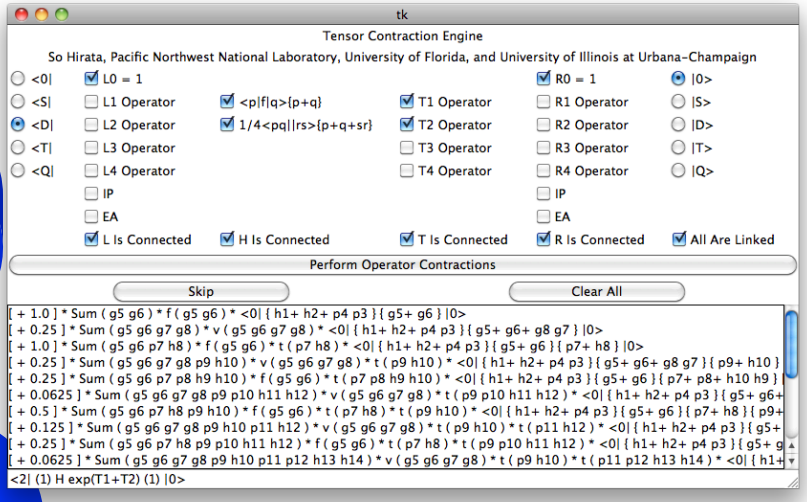
Systematic many-body methods



Automated symbolic algebra

Definition of a many-electron theory

$$E = \langle \Phi_0 | \left[e^{-T_1-T_2} H e^{T_1+T_2} \right]_C | \Phi_0 \rangle; \quad 0 = \langle \Phi_i^a | \left[e^{-T_1-T_2} H e^{T_1+T_2} \right]_C | \Phi_0 \rangle; \quad 0 = \langle \Phi_{ij}^{ab} | \left[e^{-T_1-T_2} H e^{T_1+T_2} \right]_C | \Phi_0 \rangle$$

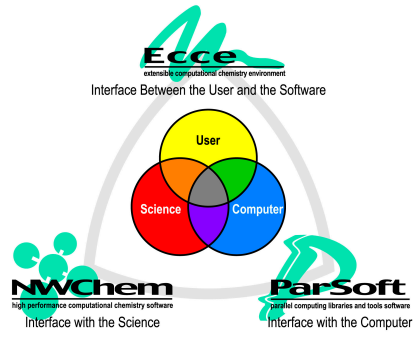


Mathematical expressions

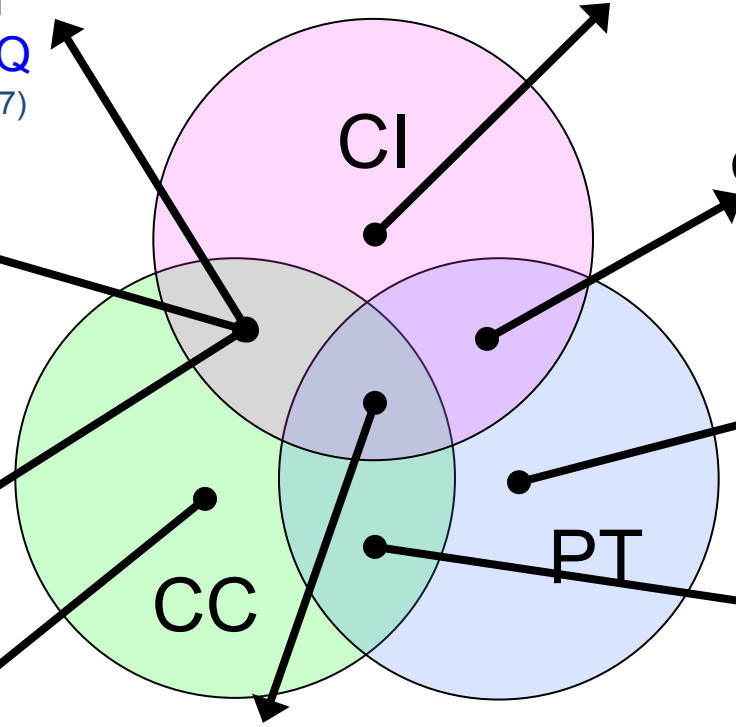
$$(\Xi_1)_{h_1p_9}^{h_7h_{10}} = +t_{h_1}^{p_5} v_{p_5p_9}^{h_7h_{10}}$$
$$(\Xi_2)_{h_1h_2}^{h_{10}h_{11}} = -\tfrac{1}{2} t_{h_1h_2}^{p_7p_8} v_{p_7p_8}^{h_{10}h_{11}}$$
$$(\Xi_3)_{h_1p_5}^{h_{10}p_3} = -\tfrac{1}{2} t_{h_1}^{p_6} v_{p_5p_6}^{h_{10}p_3}$$
$$(\Xi_4)_{p_5}^{h_{10}} = -t_{h_7}^{p_6} v_{p_5p_6}^{h_7h_{10}}$$
$$(\xi_{222})_{h_1p_5}^{h_{10}h_{11}} = +v_{h_1p_5}^{h_{10}h_{11}} + \tfrac{1}{2} (\Xi_1)_{h_1p_5}^{h_{10}h_{11}}$$
$$(\xi_{22})_{h_1h_2}^{h_{10}h_{11}} = -v_{h_1h_2}^{h_{10}h_{11}} + P_2 t_{h_1}^{p_5} (\xi_{222})_{h_2p_5}^{h_{10}h_{11}} + (\Xi_2)_{h_1h_2}^{h_{10}h_{11}}$$
$$(\xi_{23})_{h_1p_5}^{h_{10}p_3} = +v_{h_1p_5}^{h_{10}p_3} + (\Xi_3)_{h_1p_5}^{h_{10}p_3}$$
$$(\xi_{24})_{p_5}^{h_{10}} = +f_{p_5}^{h_{10}} + (\Xi_4)_{p_5}^{h_{10}}$$
$$(\xi_{25})_{h_1p_9}^{h_7h_{10}} = +v_{h_1p_9}^{h_7h_{10}} + (\Xi_1)_{h_1p_9}^{h_7h_{10}}$$
$$(\xi_2)_{h_1h_2}^{h_{10}p_3} = +v_{h_1h_2}^{h_{10}p_3} + \tfrac{1}{2} t_{h_{11}}^{p_3} (\xi_{22})_{h_1h_2}^{h_{10}h_{11}} - P_2 t_{h_1}^{p_5} (\xi_{23})_{h_2p_5}^{h_{10}p_3}$$
$$-t_{h_1h_2}^{p_3p_5} (\xi_{24})_{p_5}^{h_{10}} + P_2 t_{h_1h_7}^{p_3p_9} (\xi_{25})_{h_2p_9}^{h_7h_{10}} + \tfrac{1}{2} t_{h_1h_2}^{p_5p_6} v_{p_5p_6}^{h_{10}p_3}$$
$$(\xi_3)_{h_1p_5}^{p_3p_4} = +v_{h_1p_5}^{p_3p_4} - \tfrac{1}{2} t_{h_1}^{p_6} v_{p_5p_6}^{p_3p_4}$$
$$(\xi_{42})_{p_8}^{h_9} = +f_{p_8}^{h_9} + (\Xi_4)_{p_8}^{h_9}$$
$$(\xi_4)_{h_1}^{h_9} = +f_{h_1}^{h_9} + t_{h_1}^{p_8} (\xi_{42})_{p_8}^{h_9} - t_{h_7}^{p_6} v_{h_1p_6}^{h_7h_9} - \tfrac{1}{2} t_{h_1h_8}^{p_6p_7} v_{p_6p_7}^{h_8h_9}$$
$$(\xi_5)_{p_5}^{p_3} = +f_{p_5}^{p_3} - t_{h_7}^{p_6} v_{p_5p_6}^{h_7p_3} - \tfrac{1}{2} t_{h_7h_8}^{p_3p_6} v_{p_5p_6}^{h_7h_8}$$
$$(\xi_{62})_{h_1p_8}^{h_9h_{11}} = +v_{h_1p_8}^{h_9h_{11}} + \tfrac{1}{2} (\Xi_1)_{h_1p_8}^{h_9h_{11}}$$
$$(\xi_6)_{h_1h_2}^{h_9h_{11}} = -v_{h_1h_2}^{h_9h_{11}} + P_2 t_{h_1}^{p_8} (\xi_{62})_{h_2p_8}^{h_9h_{11}} + (\Xi_2)_{h_1h_2}^{h_9h_{11}}$$
$$(\xi_7)_{h_1p_5}^{h_6p_3} = +v_{h_1p_5}^{h_6p_3} + 2 (\Xi_3)_{h_1p_5}^{h_6p_3} - \tfrac{1}{2} t_{h_1h_8}^{p_3p_7} v_{p_5p_7}^{h_6h_8}$$
$$r_{h_1h_2}^{p_3p_4} = +v_{h_1h_2}^{p_3p_4} - P_2 t_{h_{10}}^{p_3} (\xi_2)_{h_1h_2}^{h_{10}p_4} - P_2 t_{h_1}^{p_5} (\xi_3)_{h_2p_5}^{p_3p_4} - P_2 t_{h_1h_9}^{p_3p_4} (\xi_4)_{h_2}^{h_9} + P_2 t_{h_1h_2}^{p_3p_5} (\xi_5)_{p_5}^{p_4}$$
$$-\tfrac{1}{2} t_{h_9h_{11}}^{p_3p_4} (\xi_6)_{h_1h_2}^{h_9h_{11}} - P_4 t_{h_1h_6}^{p_3p_5} (\xi_7)_{h_2p_5}^{h_6p_4} + \tfrac{1}{2} t_{h_1h_2}^{p_5p_6} v_{p_5p_6}^{p_3p_4}$$

A parallel computer program

```
nprocs = GA_NNODES()
count = 0
next = NXTVAL(nprocs)
DO p3b = noab+1,noab+nvab
DO h6b = 1,noab
DO h1b = 1,noab
DO p5b = noab+1,noab+nvab
IF (next.eq.count) THEN
 IF ((.not.restricted).or.(int_mb(k_spin+p
&)+int_mb(k_spin+h1b-1)+int_mb(k_spin+p5b-
 IF (int_mb(k_spin+p3b-1)+int_mb(k_spin+h6
&1b-1)+int_mb(k_spin+p5b-1)) THEN
 IF (ieor(int_mb(k_sym+p3b-1),ieor(int_mb(
&k_sym+h1b-1),int_mb(k_sym+p5b-1)))) .eq.
&EN
 DO p7b = noab+1,noab+nvab
 DO h8b = 1,noab
 IF (int_mb(k_spin+p3b-1)+int_mb(k_spin+p7
&1b-1)+int_mb(k_spin+h8b-1)) THEN
 IF (ieor(int_mb(k_sym+p3b-1),ieor(int_mb(
&k_sym+h1b-1),int_mb(k_sym+h8b-1)))) .eq.
 IF ((restricted).and.(int_mb(k_spin+p3b-1
&t_mb(k_spin+h1b-1)+int_mb(k_spin+h8b-1).e
```



Implemented methods



Electron Attachment Theory
EA-EOM-CCSD
EA-EOM-CCSDT
EA-EOM-CCSDTQ
Kamiya & Hirata *JCP* (2007)

Ionization Theory
IP-EOM-CCSD
IP-EOM-CCSDT
IP-EOM-CCSDTQ
Kamiya & Hirata *JCP* (2006)

Excited State Theories
EOM-CCSD
EOM-CCSDT
EOM-CCSDTQ
Hirata *JCP* (2004)

Cluster Expansion
CCD, CCSD, CCSDT, CCSDTQ, LCCD, LCCSD, QCISD
Hirata *JPCA* (2003)

Linear Expansion
CIS, CISD, CISDT, CISDTQ
Hirata *JPCA* (2003)

CIS+perturbation
CIS(D), CIS(3), CIS(4)
Hirata *JCP* (2005)

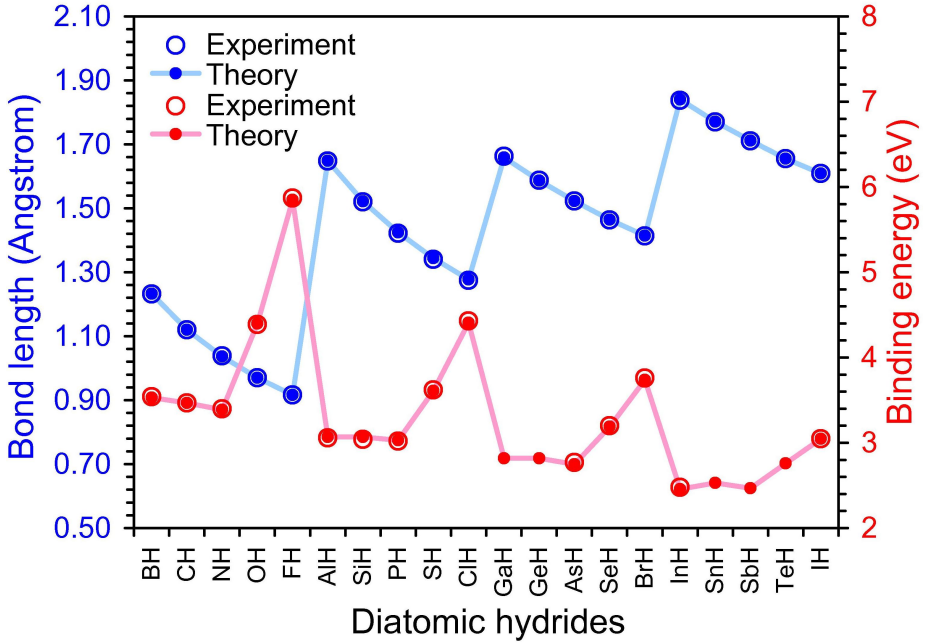
Perturbation
MP2, MP3, MP4
Hirata *JPCA* (2003)

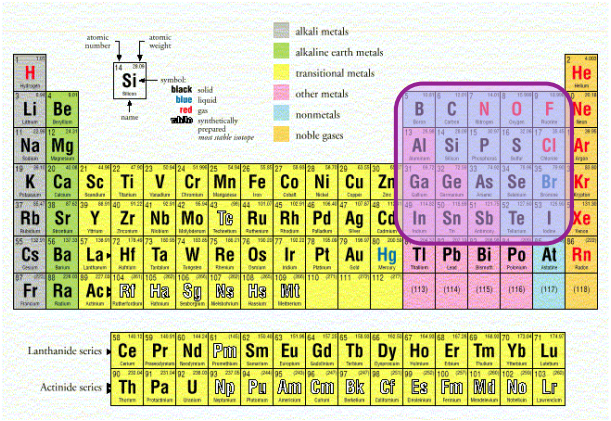
Combined CC+PT
CCSD(T)
$CCSD(2)_T$, $CCSD(3)_T$
$CCSD(2)_{TQ}$, $CCSD(3)_{TQ}$
$CCSDT(2)_Q$, CR-CCSD(T)
Hirata *et al. JCP* (2004)
Shiozaki *et al. JCP* (2007)

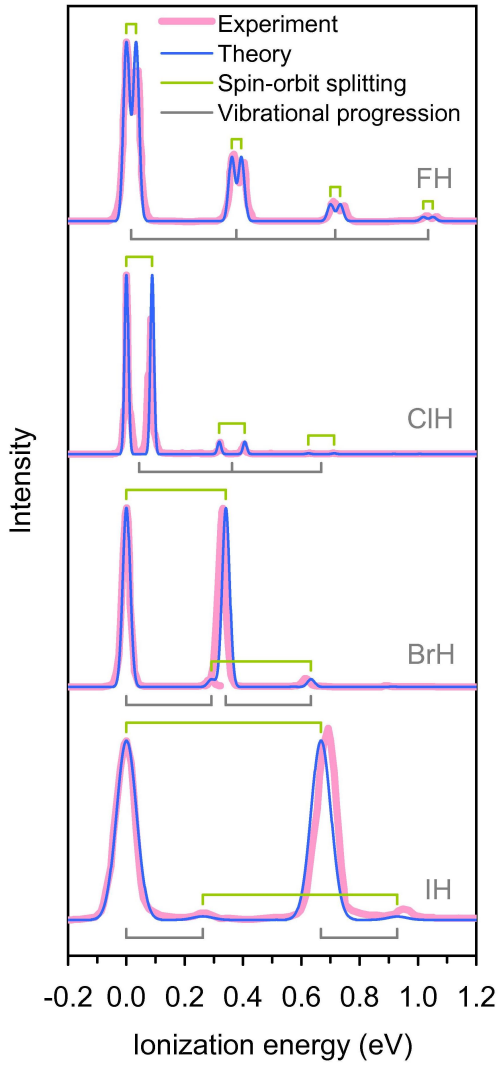
EOM-CC+perturbation
$EOM\text{-}CCSD(2)_T$, $EOM\text{-}CCSD(2)_{TQ}$
$EOM\text{-}CCSD(3)_T$
Shiozaki *et al. JCP* (2007)

Structures, thermochemistry, and spectra

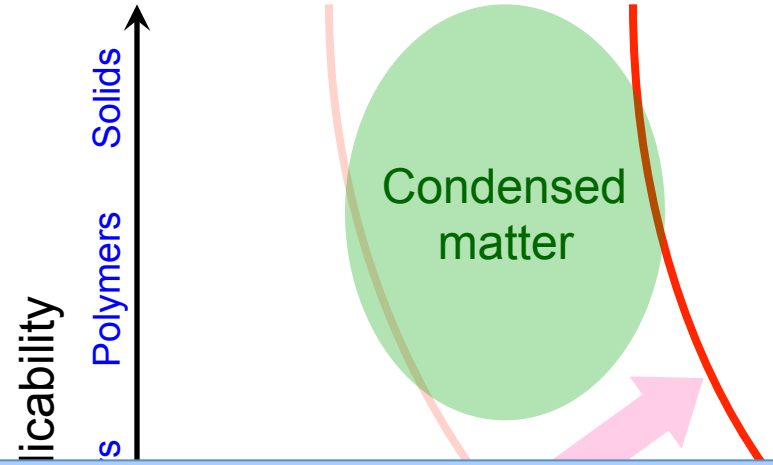
Hirata *et al.*, *J. Chem. Phys.* (2004); Hirata *et al.*, *J. Chem. Phys.* (2007)







Frontiers of predictive computing



Solid-state chemistry
Condensed matter physics
Materials science
Geochemistry
High-pressure chemistry
Planetary science
High-T_c superconductivity

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**"*

SciDAC
Scientific Discovery through Advanced Computing

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.

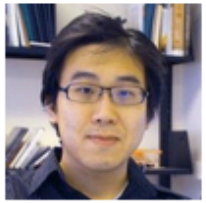
Peter Abbamonte (Physics, UIUC)

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)

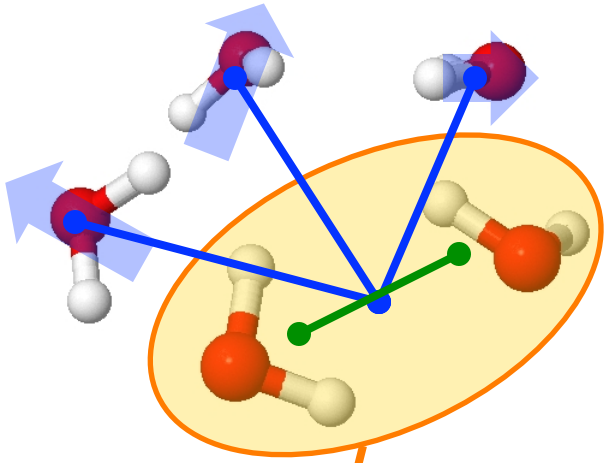
Zhang specializes in computational condensed matter physics and materials science. Zhang is a pioneer in the use of quantum Monte Carlo (QMC) in the Hilbert space for strong correlation. He is the inventor of the phaseless auxiliary field QMC.

Embedded-fragment approach

Hirata *et al.*, *Mol. Phys.* (2005); Kamiya, Hirata, and Valiev, *J. Chem. Phys.* (2008);
Hirata *et al.*, *Acc. Chem. Res.* (2014)

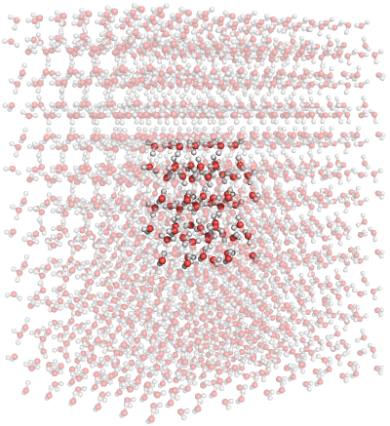
***N*-body (*N* > 2) Coulomb in point-charge or dipole approximation**

1 and 2-body
Coulomb
Exchange
Correlation



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

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

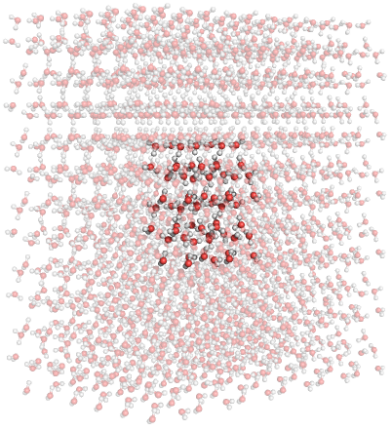


Cf. Li, Paulus, Schutz, Manby, Beran, Truhlar, Raghavachari, Herbert, Collins, Gordon, Gao, Fedorov, Kitaura, Zhang, et al.

Ice Ih

He, Sode, Xantheas, and Hirata, *J. Chem. Phys.* (2012)

Xiao He



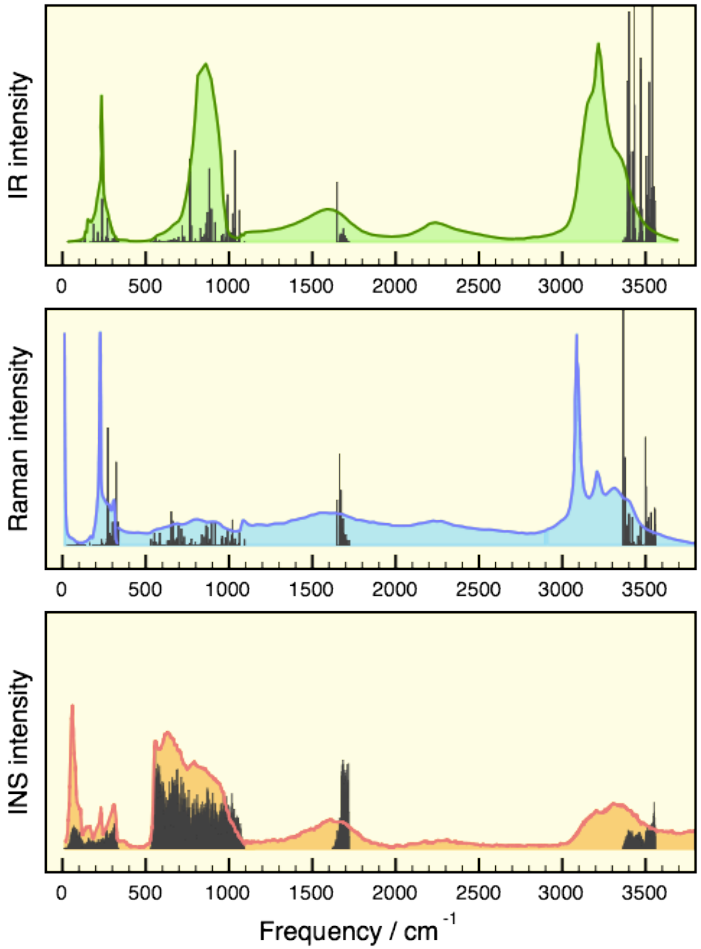
MP2/aug-cc-pVDZ

Ice Ih

He, Sode, Xantheas, and Hirata, *J. Chem. Phys.* (2012)

Xiao He

IR, Raman, and Inelastic neutron scattering spectra

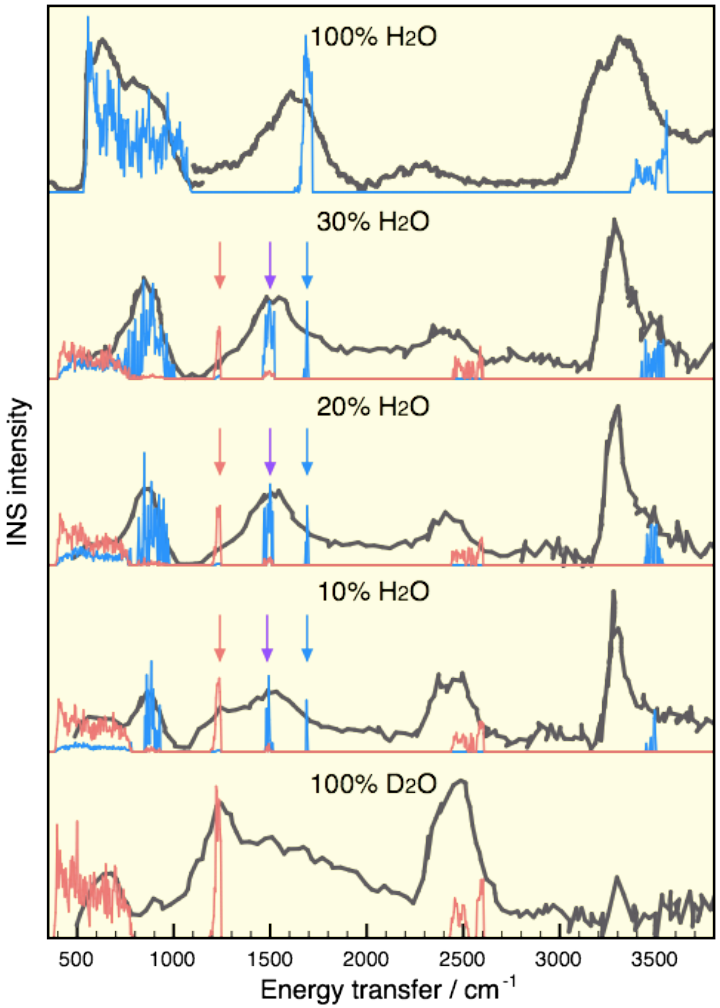


Ice Ih

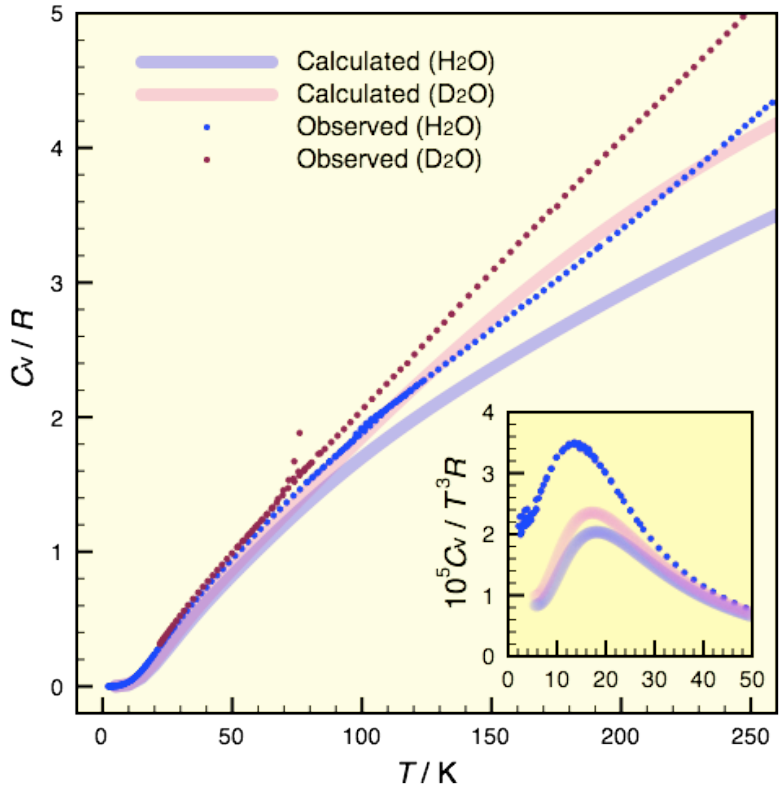
He, Sode, Xantheas, and Hirata, *J. Chem. Phys.* (2012)

Xiao He

Inelastic neutron scattering spectra



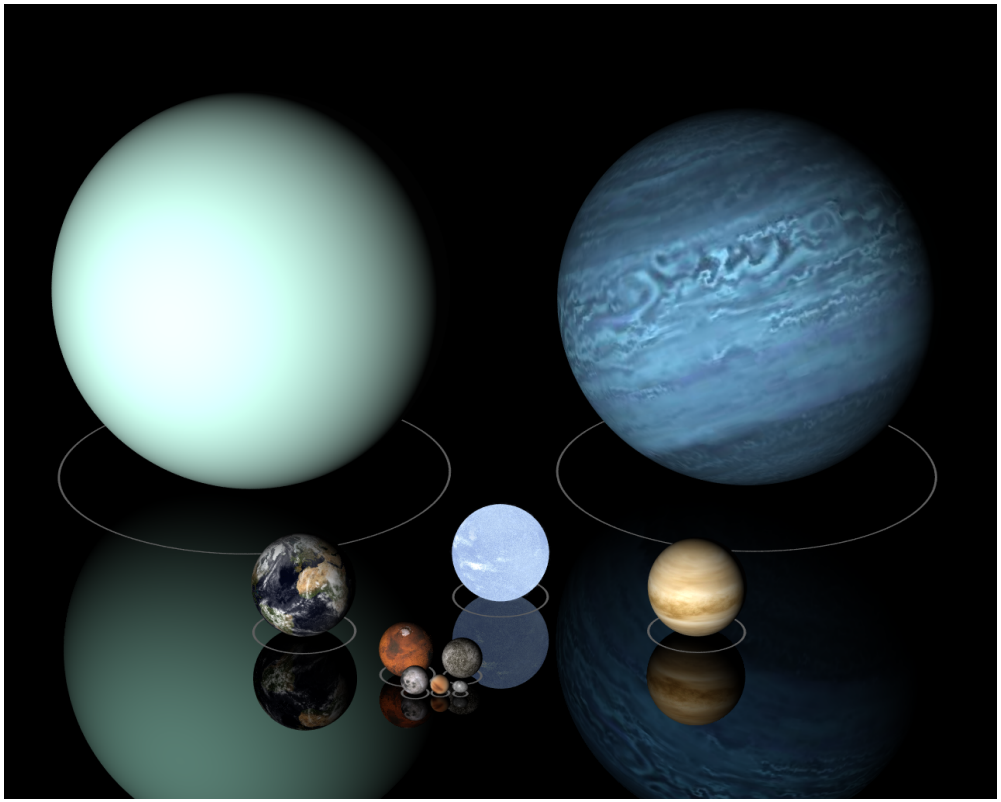
Heat capacities

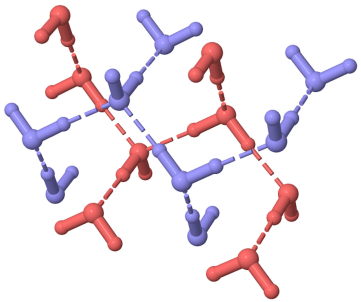


Ice VIII

Gilliard, Sode, and Hirata, *J. Chem. Phys.* (2014)

Kandis Gilliard



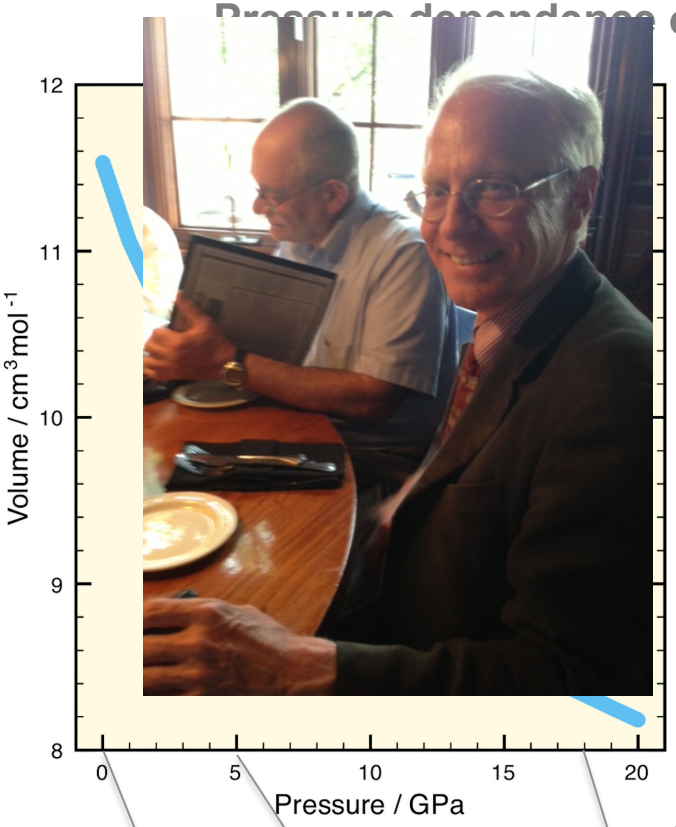


MP2/aug-cc-pVDZ
CCSD/aug-cc-pVDZ

Ice VIII

Gilliard, Sode, and Hirata, *J. Chem. Phys.* (2014)

Kandis Gilliard



Diamond synthesis (18 GPa)

Center of the Moon (5 GPa)

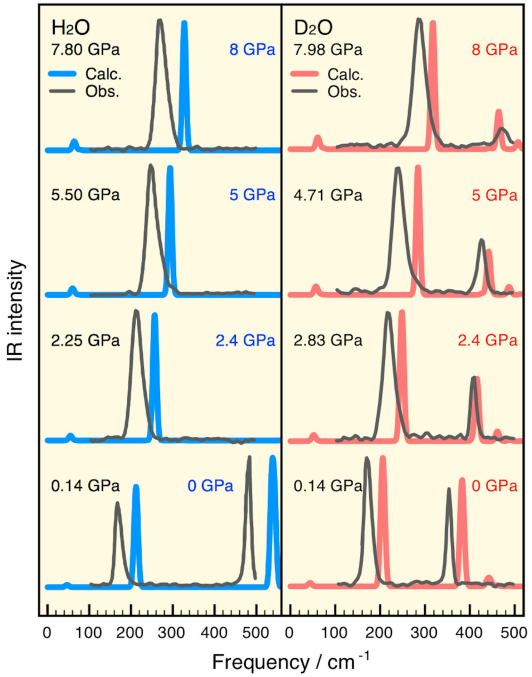
Bottom of the Mariana Trench (0.1 GPa)

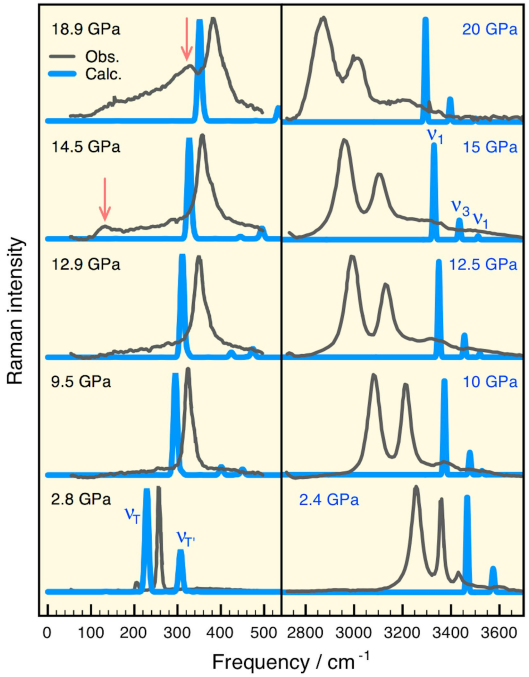
Ice VIII

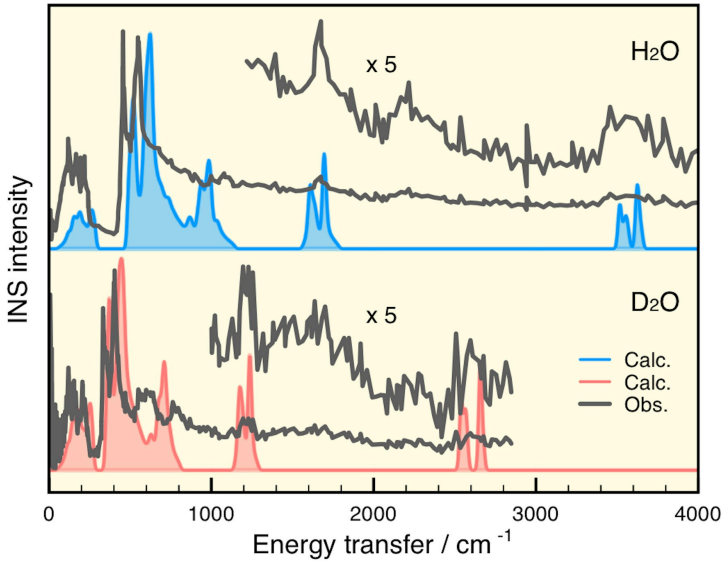
Gilliard, Sode, and Hirata, *J. Chem. Phys.* (2014)

Kandis Gilliard

Pressure dependence of IR, Raman, and INS spectra



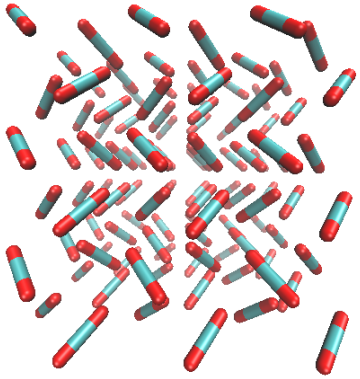




Solid CO_2

Sode, Keçeli, Yagi, and Hirata, *J. Chem. Phys.* (2012)

Olaseni Sode



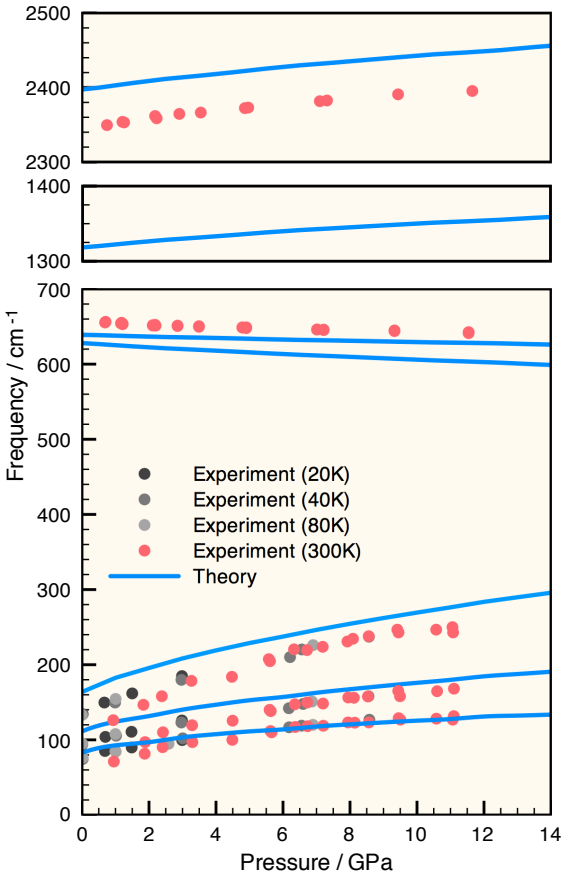
MP2/aug-cc-pVDZ

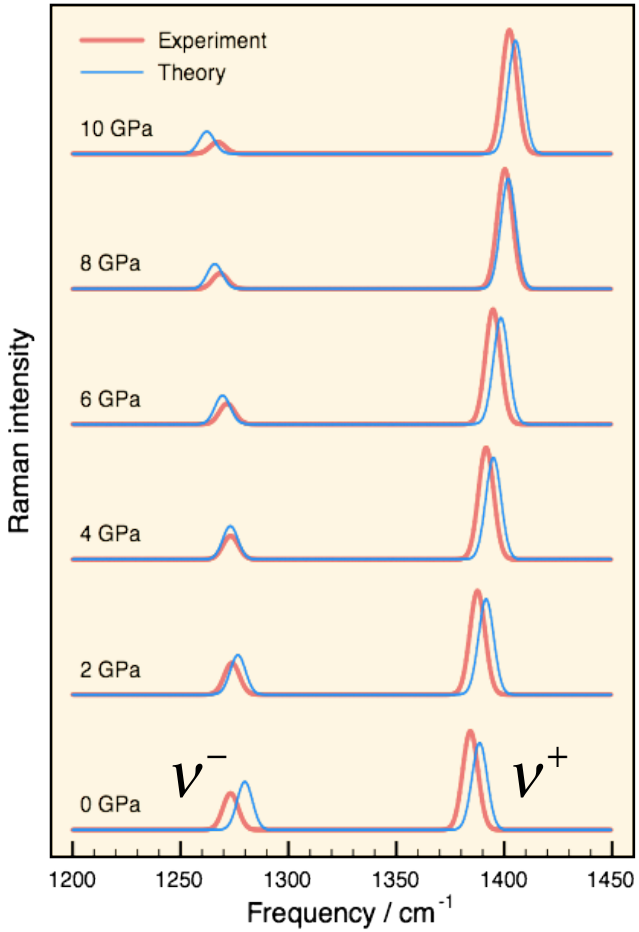
Solid CO_2

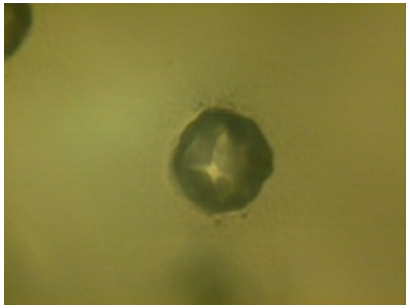
Sode, Keçeli, Yagi, and Hirata, *J. Chem. Phys.* (2012)

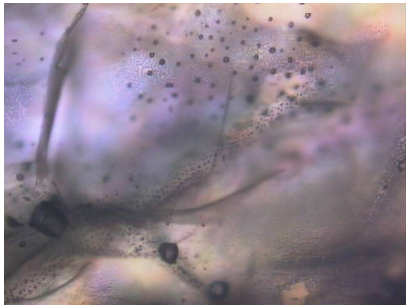
Olaseni Sode

Pressure dependence of Raman spectra





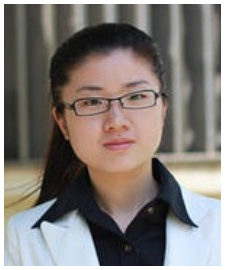




CO_2 encapsulation in minerals

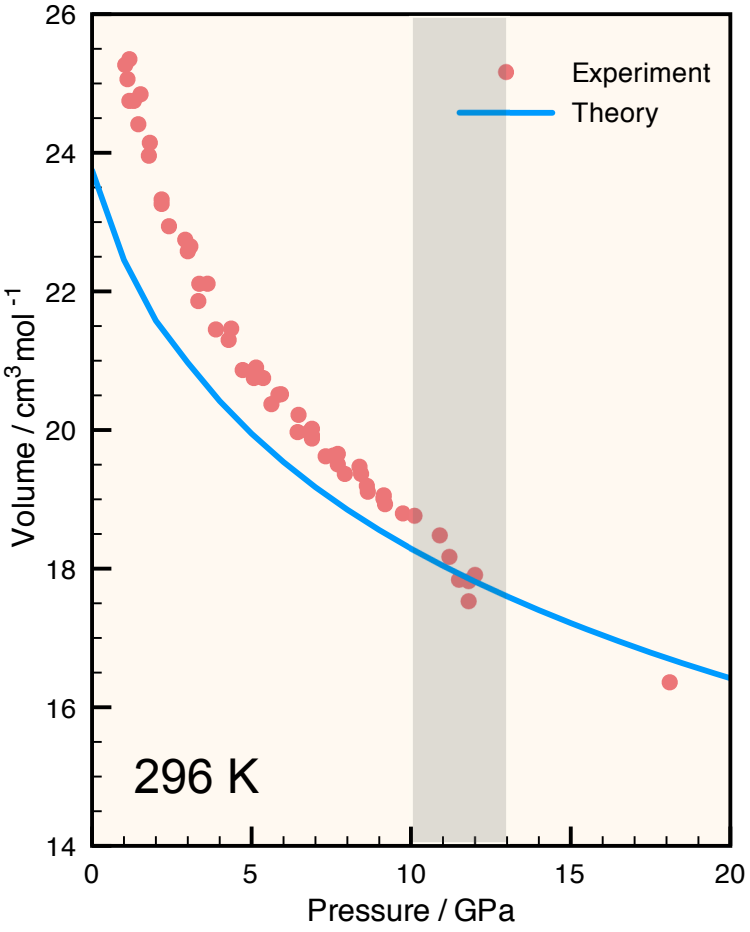
Phase transition in solid CO_2

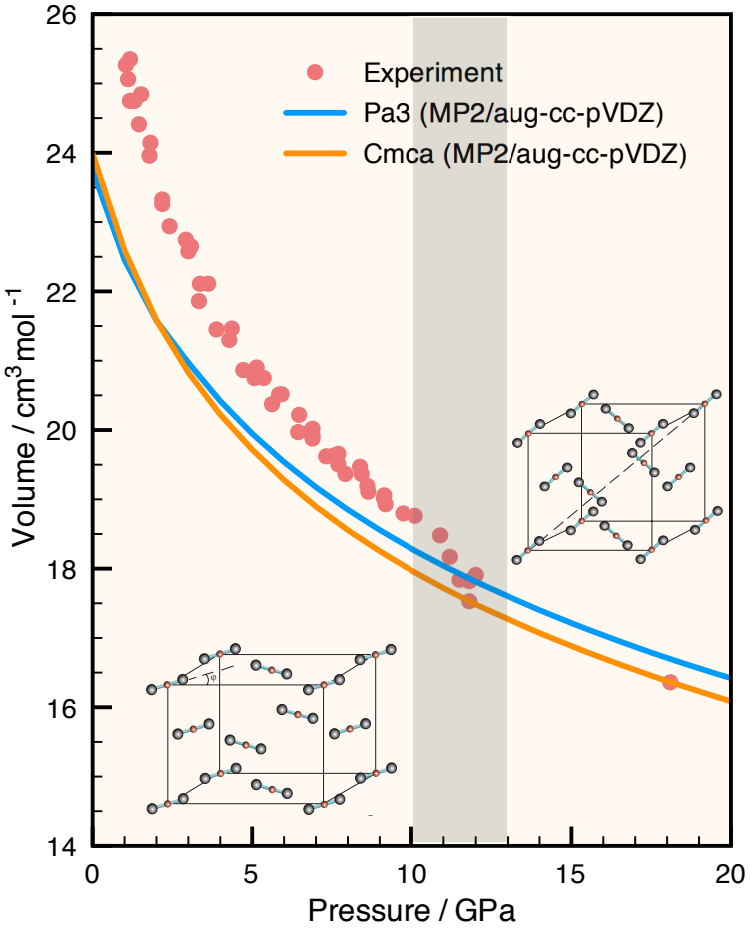
Li, Sode, Voth and Hirata, *Nature Communications* (2013)



Jinjin Li

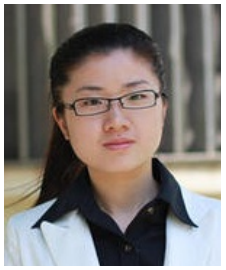
Pressure dependence of volume



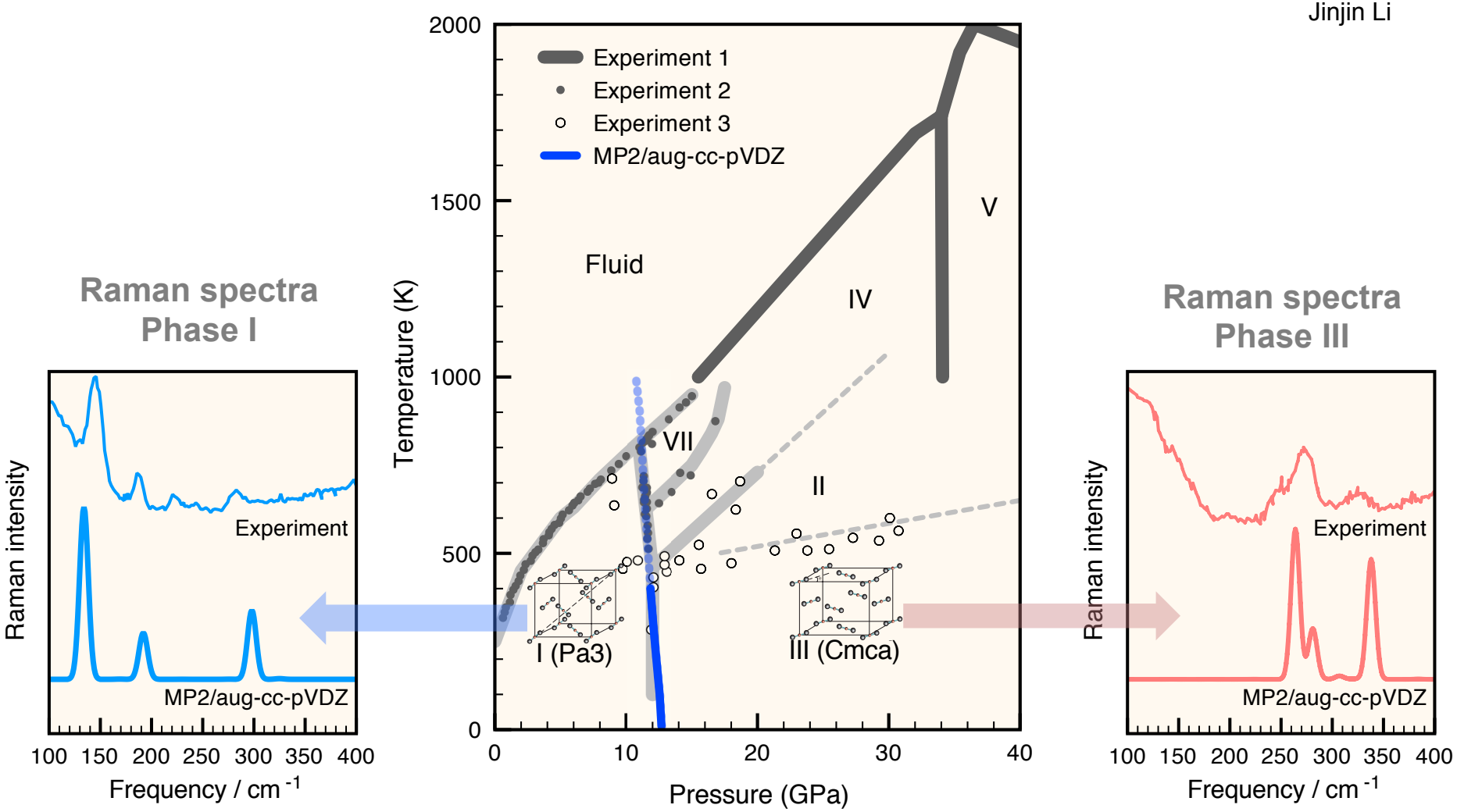


Phase transition in solid CO_2

Li, Sode, Voth and Hirata, *Nature Communications* (2013)



Jinjin Li



What can be done with Blue Waters?

- First-principles phase diagram of ice
- First-principles prediction of thermal expansion of ice
- First-principles simulation of liquid water
- First-principles simulation of chemical reactions in aqueous media

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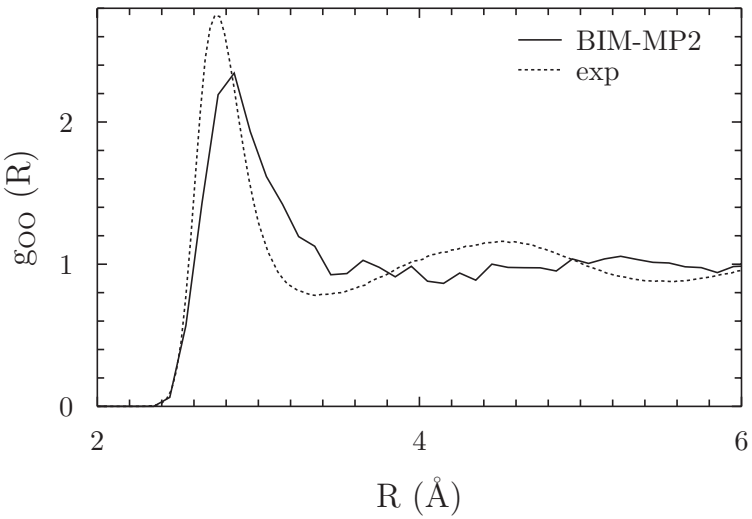

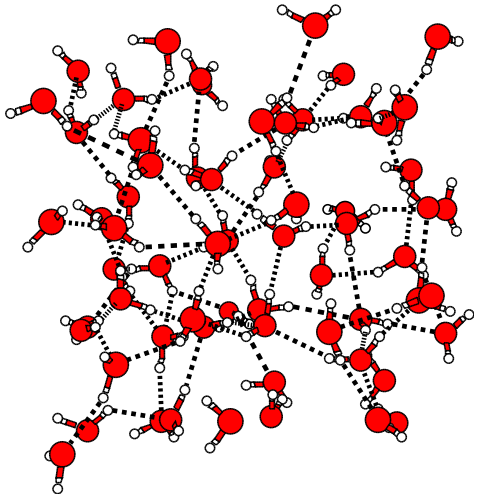

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Monte Carlo MP2

Willow, Kim and Hirata, *J. Chem. Phys.* (2012)

Very long $O(n^4)$ summation of products of two 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, *J. Chem. Phys.* (2012)

Soohaeng Willow

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

weight function

Metropolis

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

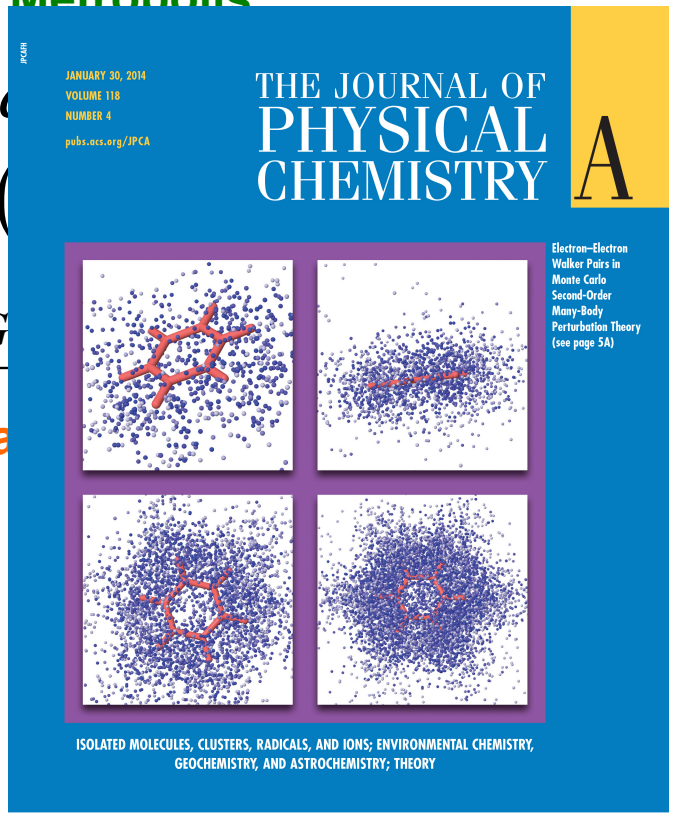
Requirement 2: **cancellation of singularities** $f($

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

Singula

$$g(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4) = \frac{1}{4E^2_{\text{Coulomb}}} \frac{\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)}{r_{12}} \frac{\rho(\mathbf{r}_3)\rho(\mathbf{r}_4)}{r_{34}}$$

$$\int g(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4)\,d\mathbf{r}_1\,d\mathbf{r}_2\,d\mathbf{r}_3\,d\mathbf{r}_4 = 1$$



MC-MP2 for E_{corr}, IP, and EA

Willow, Kim and Hirata, *J. Chem. Phys.* (2012)
Willow, Kim and Hirata, *J. Chem. Phys.* (2013)

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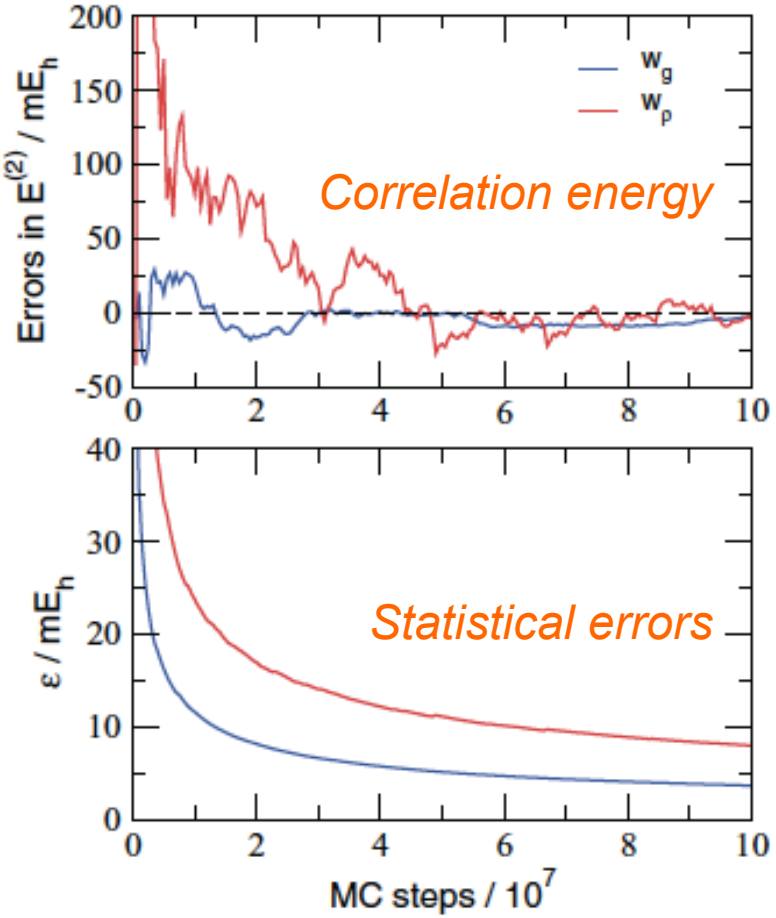
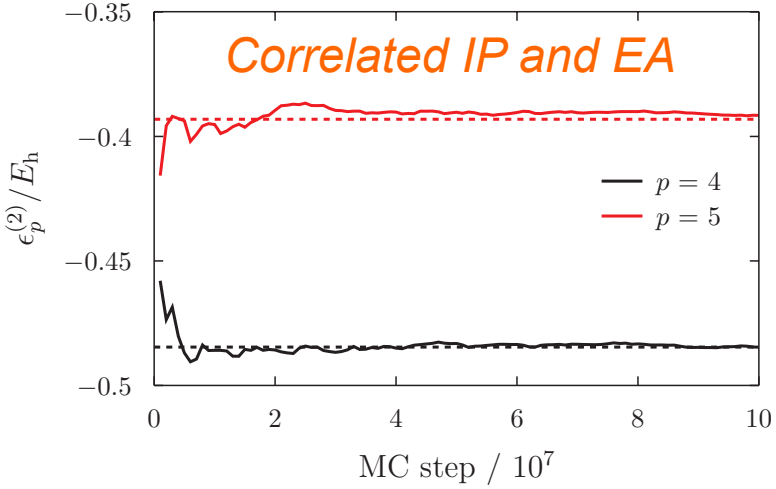
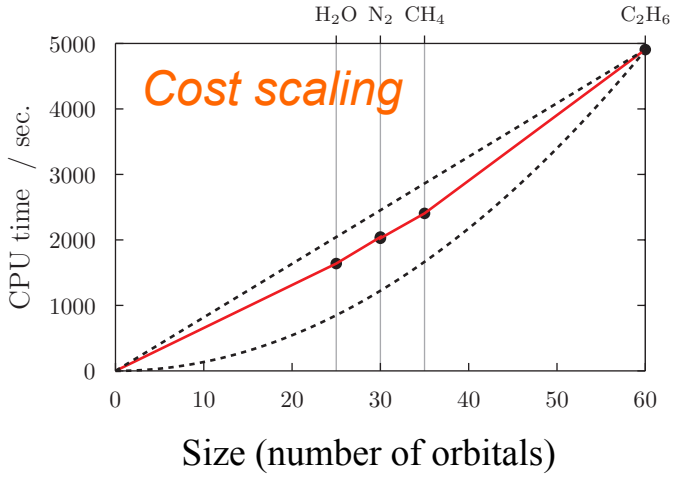
Nitrogen 6-31G**



Water HOMO and HOMO–1



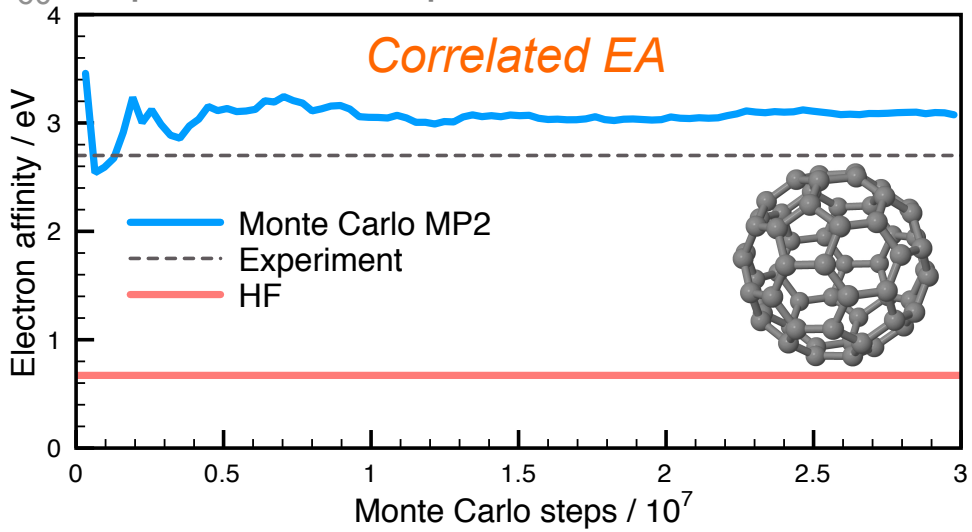


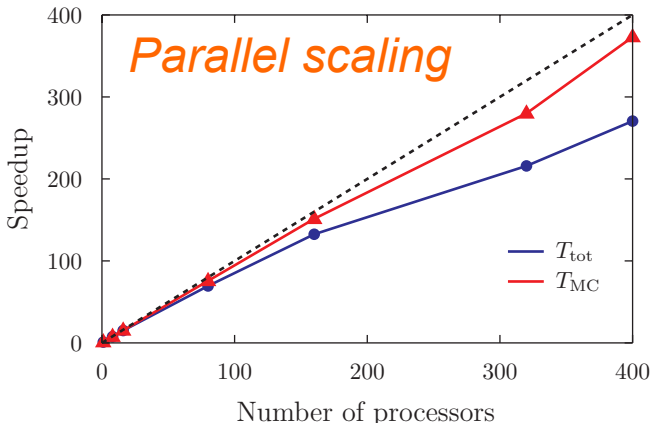
Parallel MC-MP2, MP3, MP2-R12

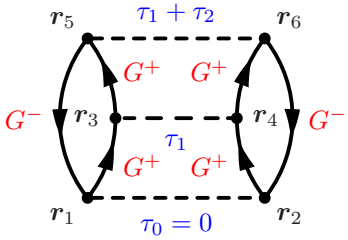
Willow, Hermes, Kim and Hirata, *J. Chem. Theo. Comput.* (2013); Willow and Hirata, *J. Chem. Phys.* (2013); Willow, Zhang, Valeev, and Hirata, *J. Chem. Phys.* (*Comm.*) (2014)

Soohaeng Willow

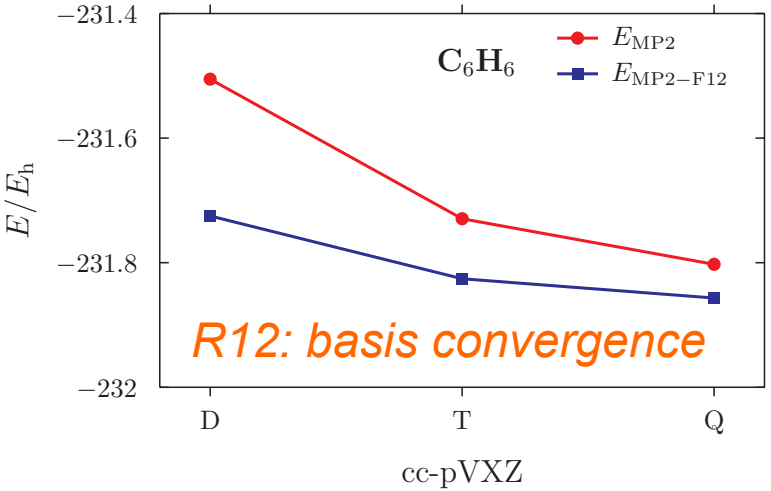
C_{60} cc-pVDZ on 320 processors of Blue Waters







Diagrammatics

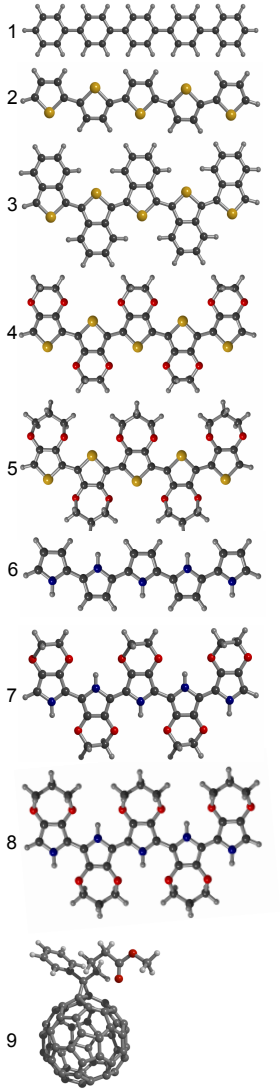


What can be done with Blue Waters?

- Accurate calculations of opto-electronic properties of conjugated polymers used in organic solar cells, LED, FET, capacitors, etc.
- Accurate calculations of van der Waals interactions between conjugated polymers, PAHs, graphene, graphite, C_{60}, etc.

Matthew Hermes

Val. band edge	PPP (1)	PT (2)
Experiment	5.2-5.65 eV	5.3-5.55 eV
DFT	5.0 eV	4.5 eV
HF	6.6 eV	6.2 eV
MP2	6.4 eV	5.5 eV



BLUE WATERS
SUSTAINED PETASCALE COMPUTING