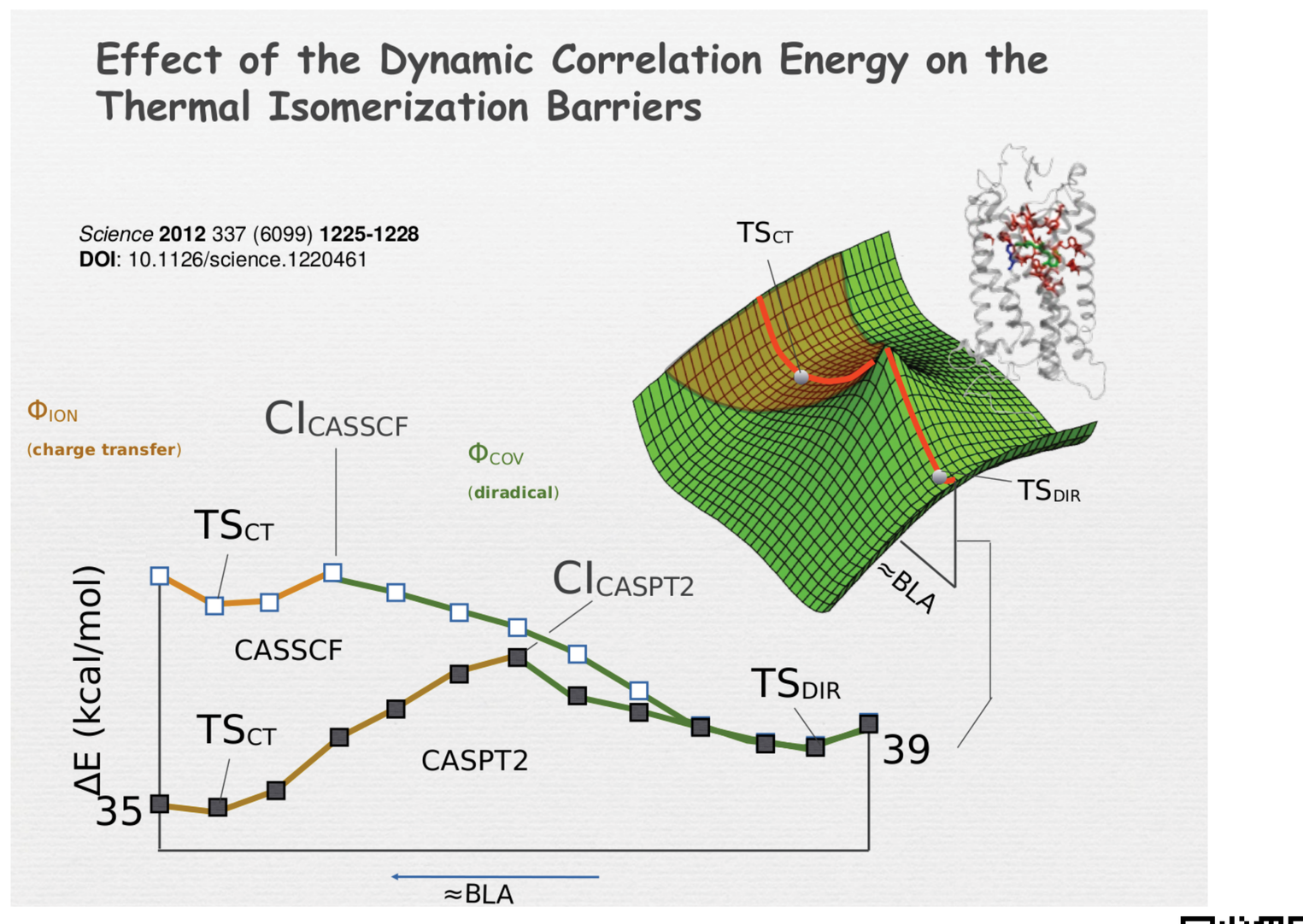
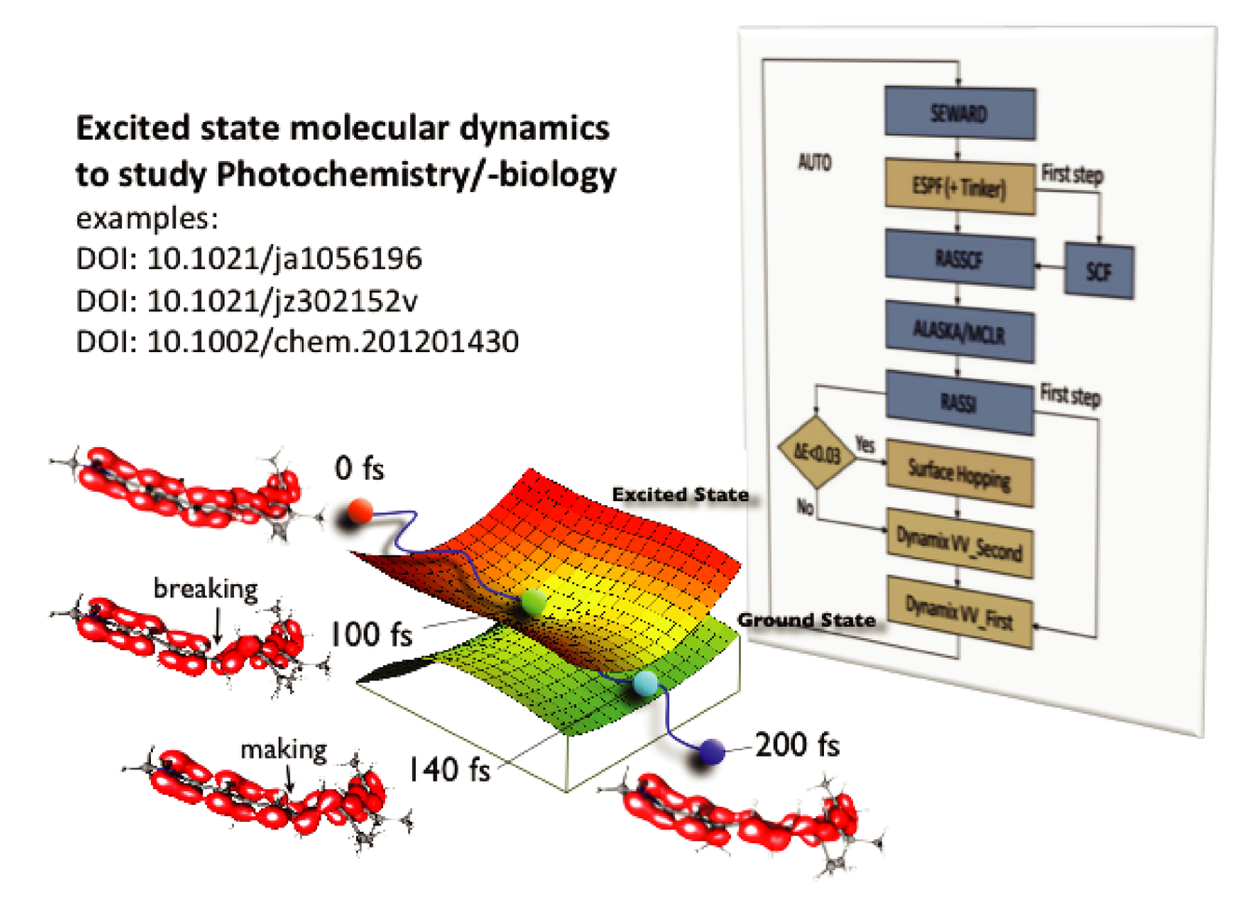
The program system MOLCAS is a package for calculations of electronic and structural properties of molecular systems in gas, liquid, or solid phase. MOLCAS contains a number of modern quantum chemical methods for studies of the electronic structure in ground and exited electronic states, including Hartree-Fock, Density Functional Theory, Coupled-Cluster, multi-configurational SCF (CASSCF and RASSCF) with dynamical electron correlation treated with multi-reference CI or second order perturbation theory (CASPT2 and RASPT2).

State of the art applications

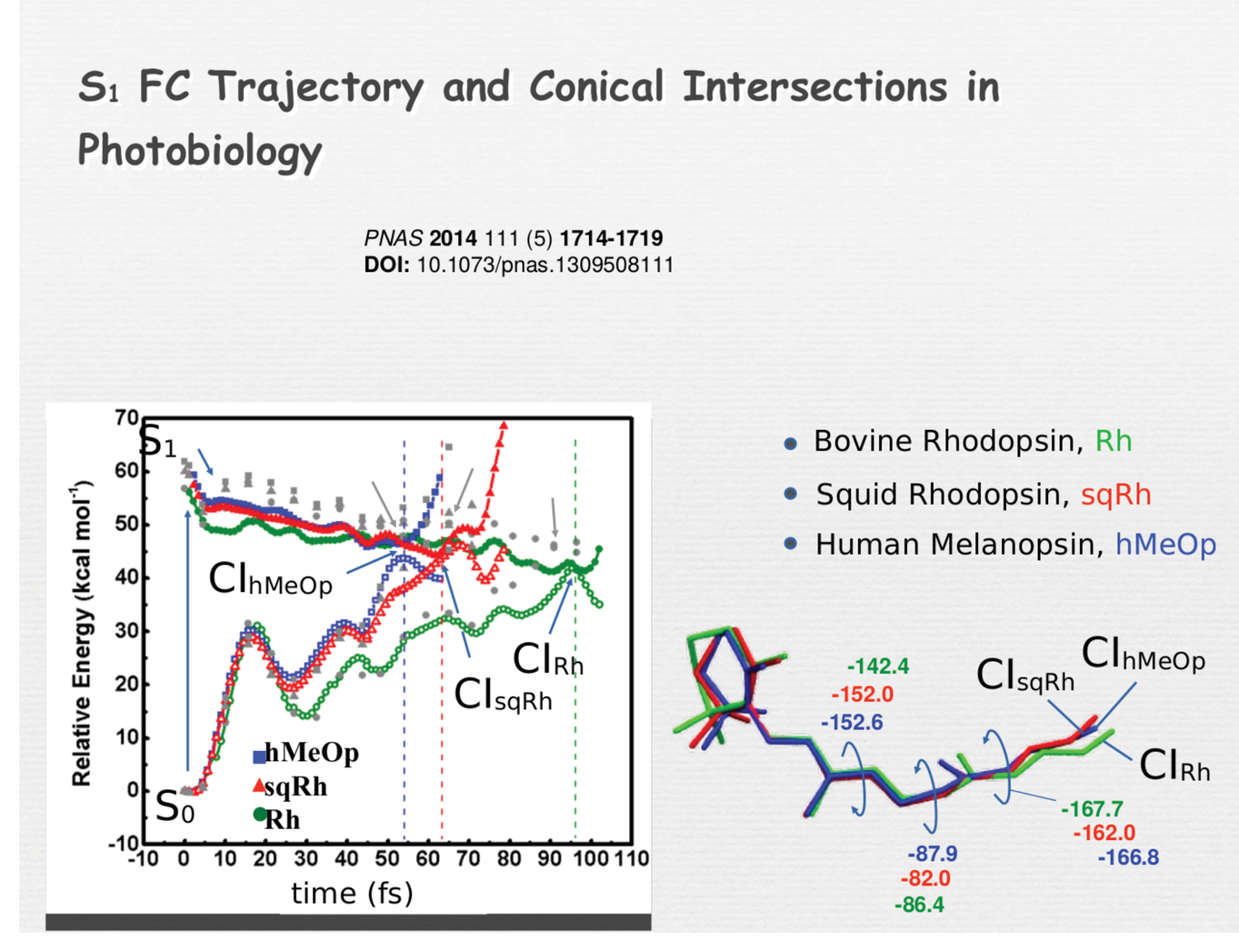


S.Gozem, I.Schapiro, N.Ferré, M.Olivucci



Excited state molecular dynamics to study Photochemistry/-biology
examples:
DOI: 10.1021/ja1056196
DOI: 10.1021/jz302152v
DOI: 10.1002/chem.201201430
0 fs
breaking
100 fs
making
140 fs
200 fs
Excited State
Ground State
SEWARD
RASSCF
ALASKA/MCLR
RASSI
Surface Hopping

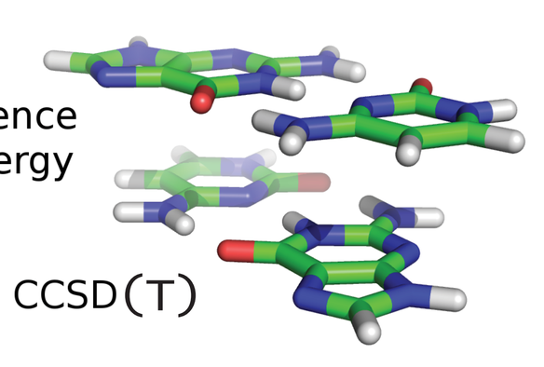
I.Schapiro

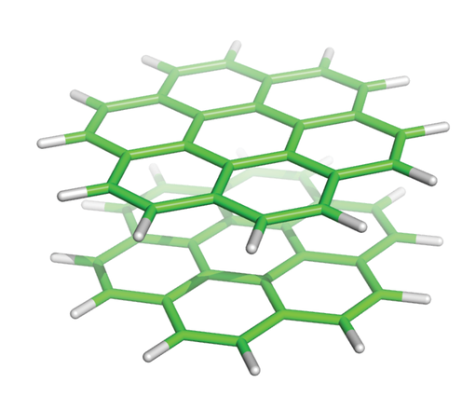


S.Rinaldi, F.Melaccio, S.Gozem, F.Fanelli, M.Olivucci

Coupled Cluster calculations

- Large-scale single-reference post-MP2 correlation energy calculations
- MP3, L-CCSD, CCSD and CCSD(T)

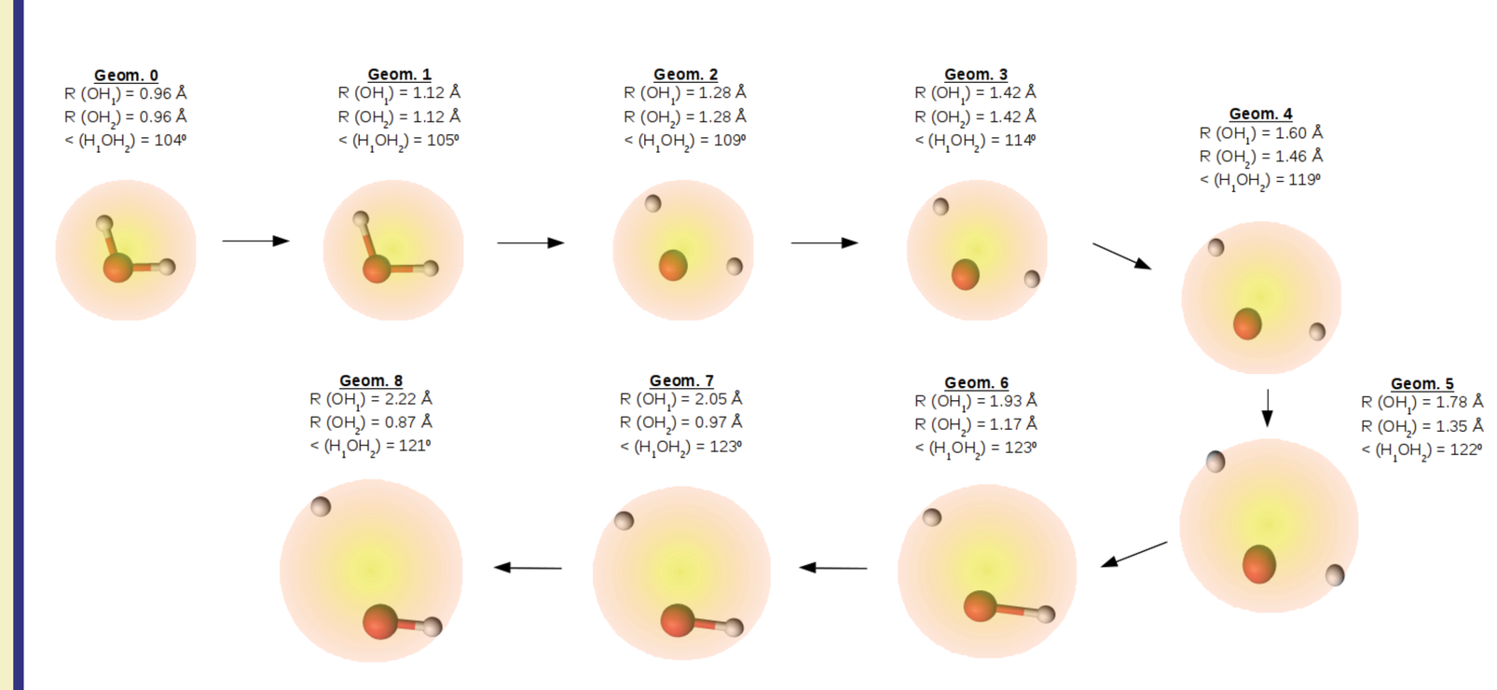




- Cholesky-decomposed 2-electron integrals based
- parallelizable to 512 nodes
- addaptable memory and storage requirements

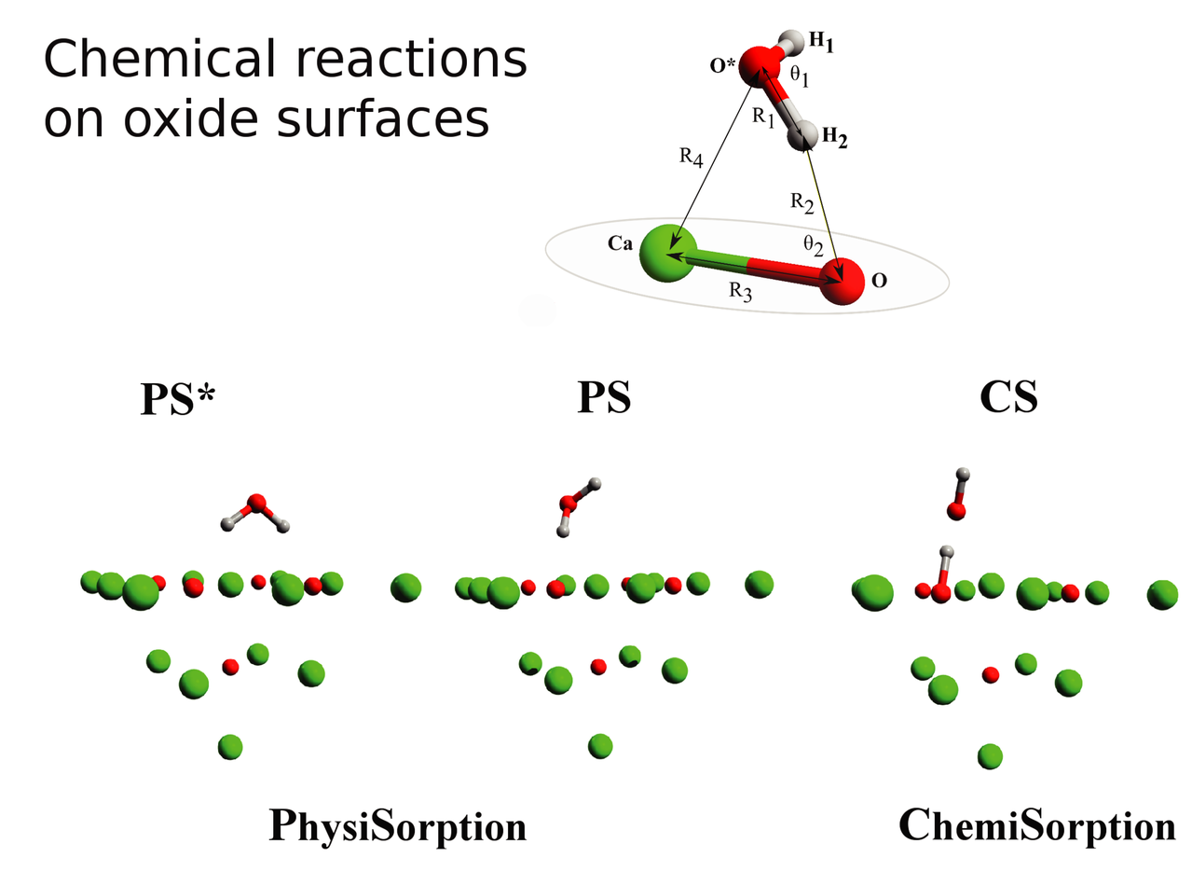
M.Pitoňák, F.Aquilante

MEP of a core excited state of water



A.Sankari, P.Å.Malmqvist

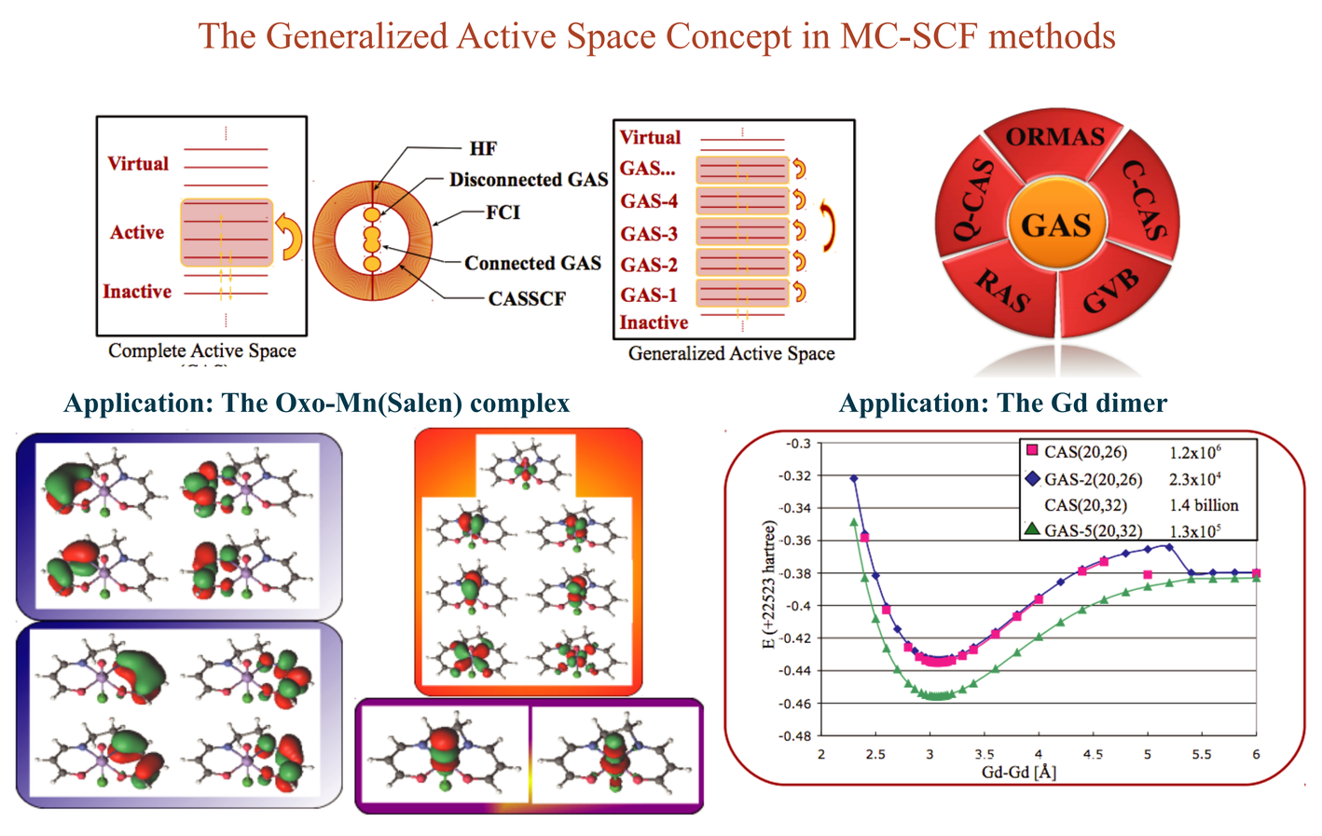
Chemical reactions on oxide surfaces



V.Vysotskiy,V.Veryazov

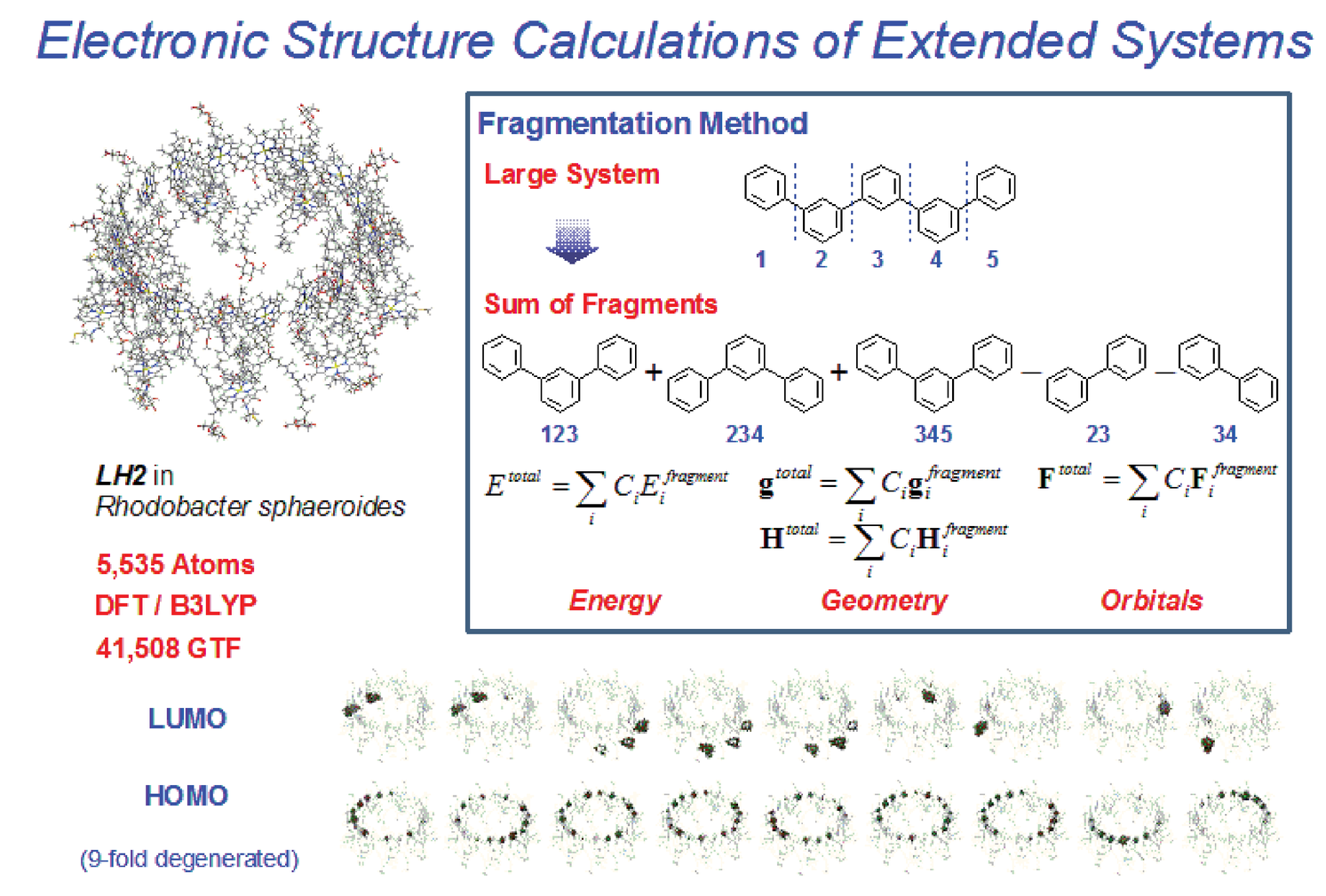
Method development

The Generalized Active Space Concept in MC-SCF methods



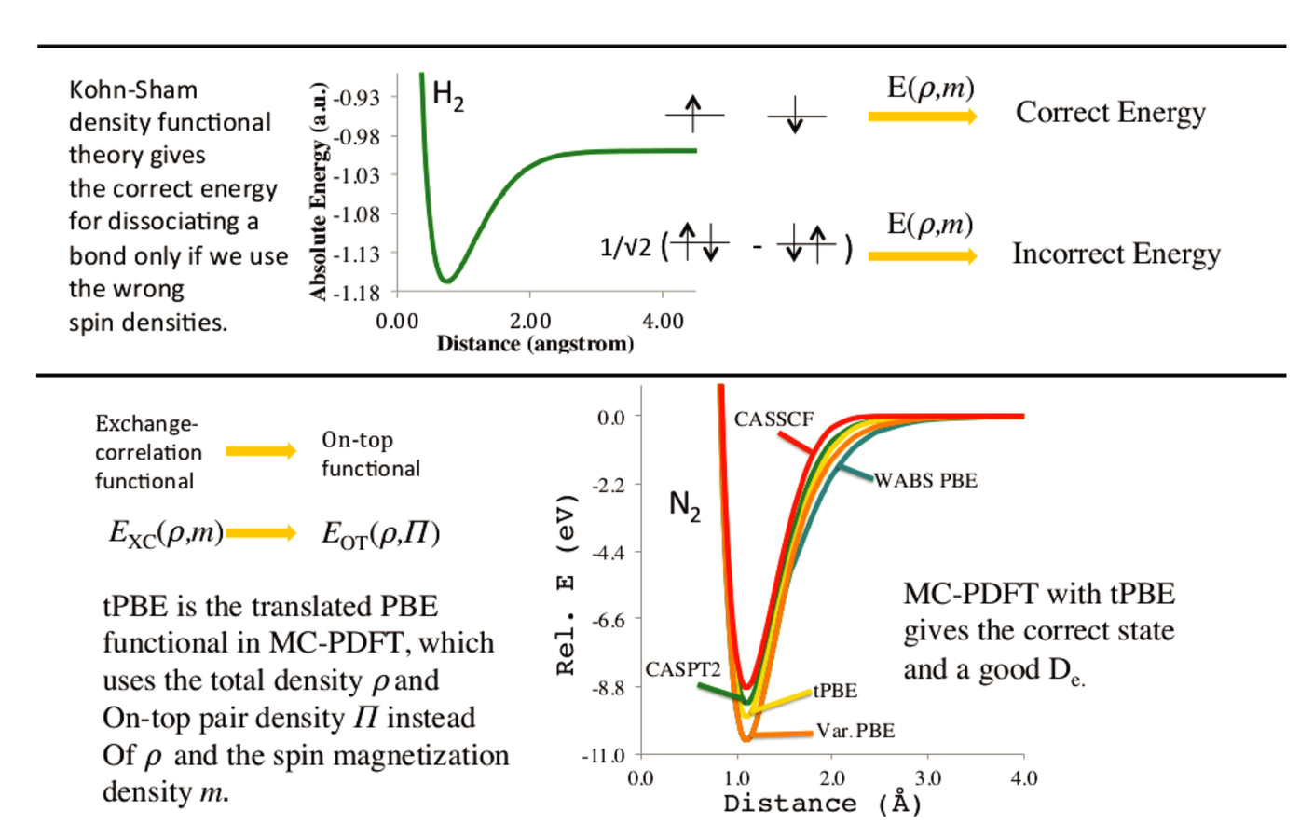
G.Li Manni, D.Ma, J.Olsen, L.Gagliardi

Electronic Structure Calculations of Extended Systems



T.Tsuchiya

Multiconfiguration pair-density functional theory

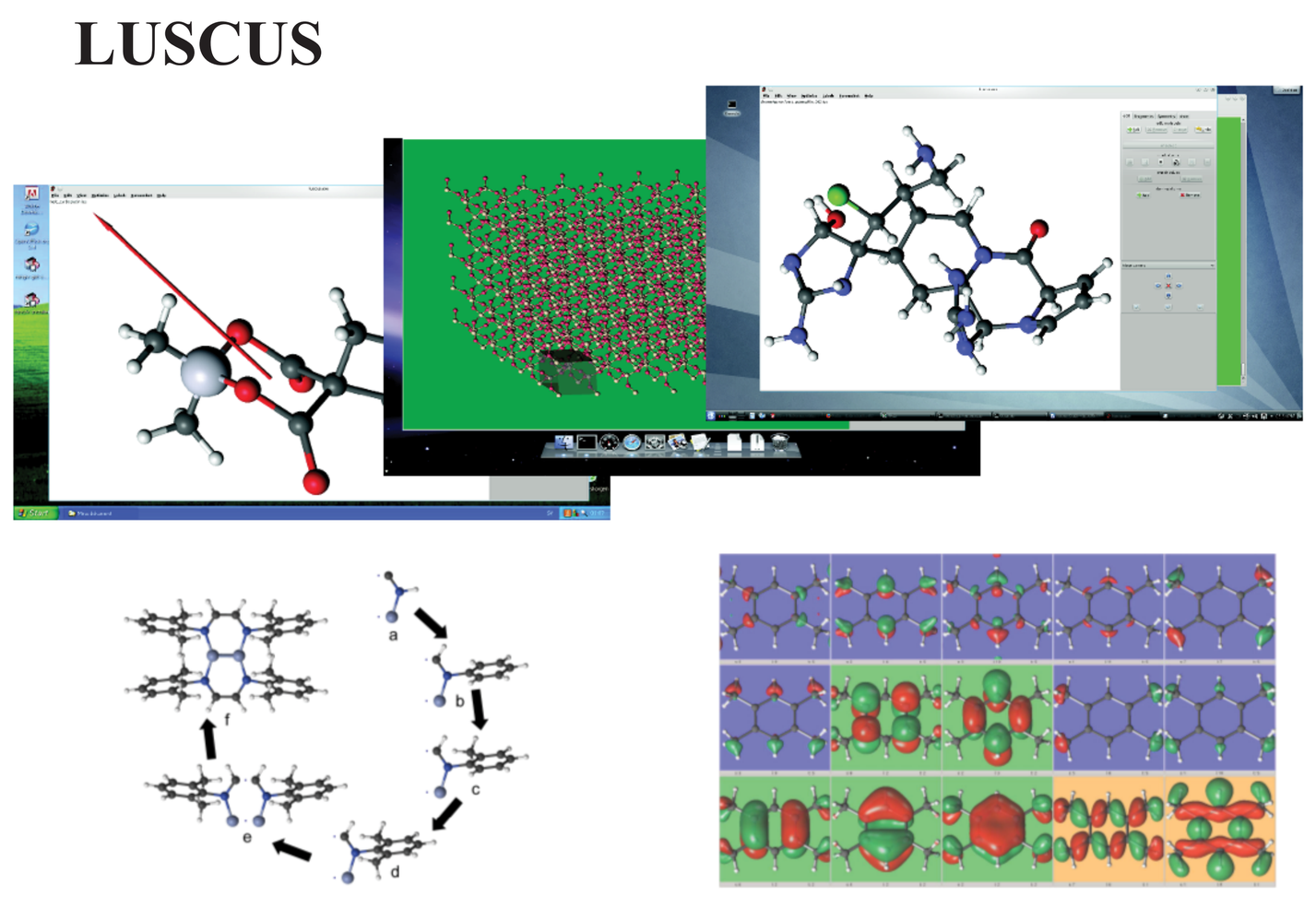


Kohn-Sham density functional theory gives the correct energy for dissociating a bond only if we use the wrong spin densities.
Correct Energy
Incorrect Energy
tPBE is the translated PBE functional in MC-PDFT, which uses the total density ρ and On-top pair density Π instead Of ρ and the spin magnetization density m.
MC-PDFT with tPBE gives the correct state and a good De.

G.Li Manni,R.K.Carlson,S.Luo,D.Ma, J.Olsen, D.G.Truhlar, L.Gagliardi

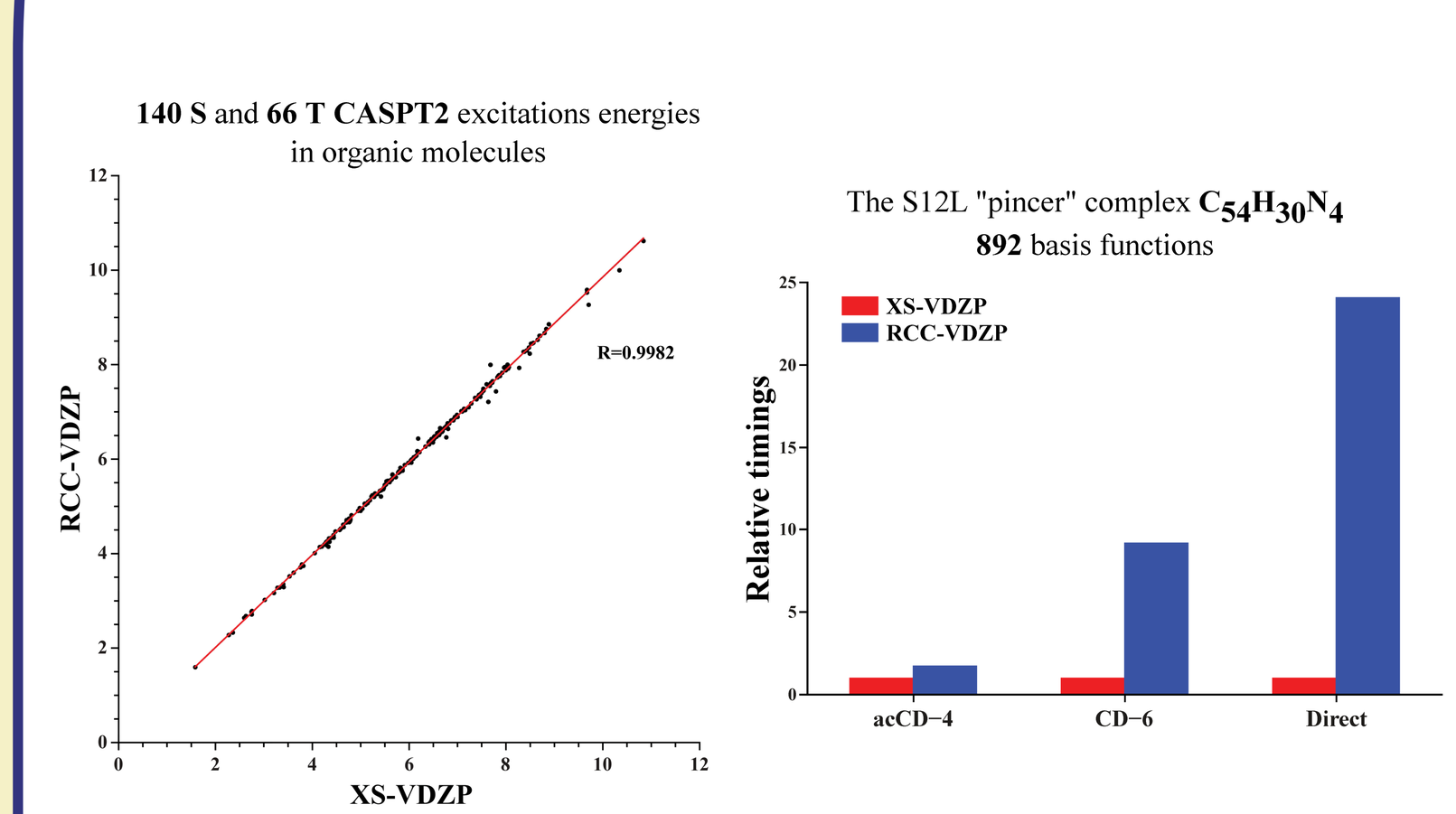
New codes and improvements

LUSCUS



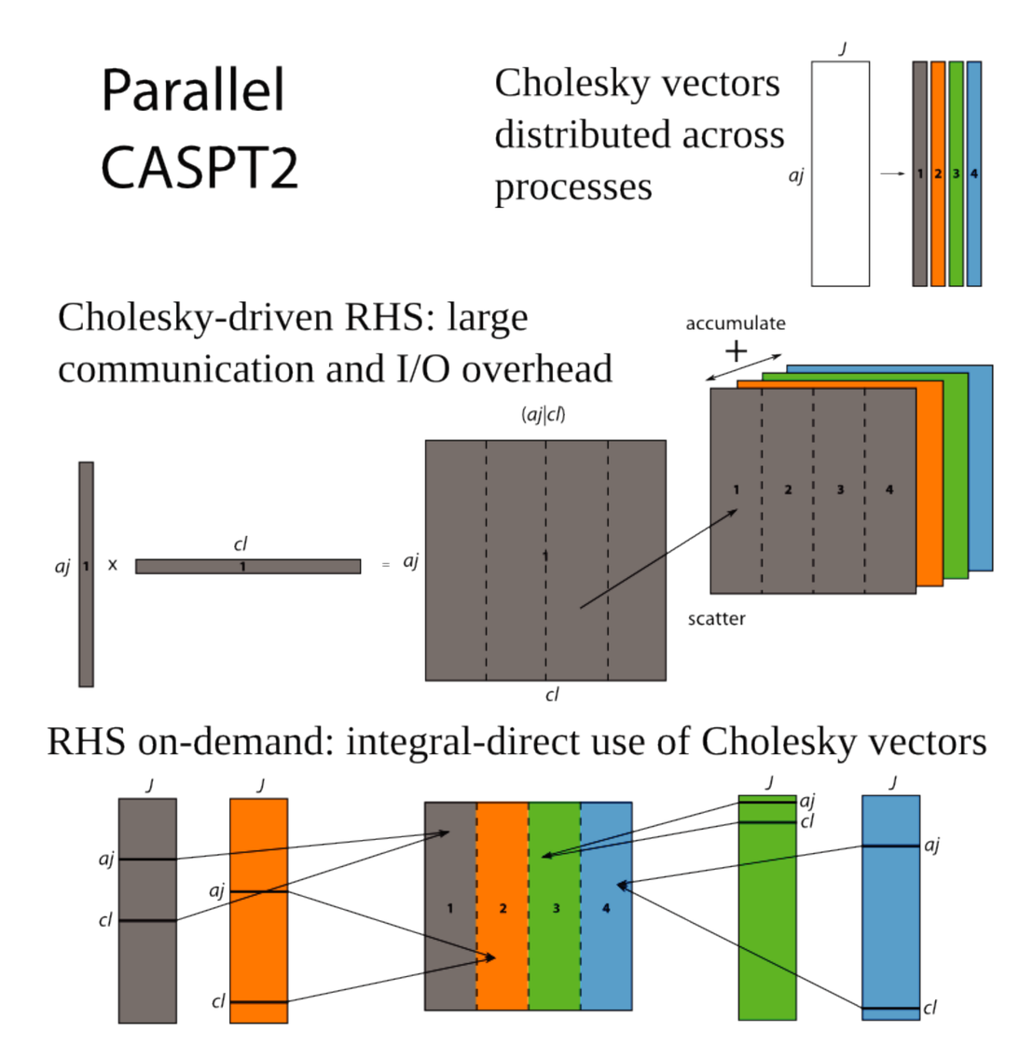
G.Kovačević, V.Veryazov

eXtra Small basis set for relativistic calculations

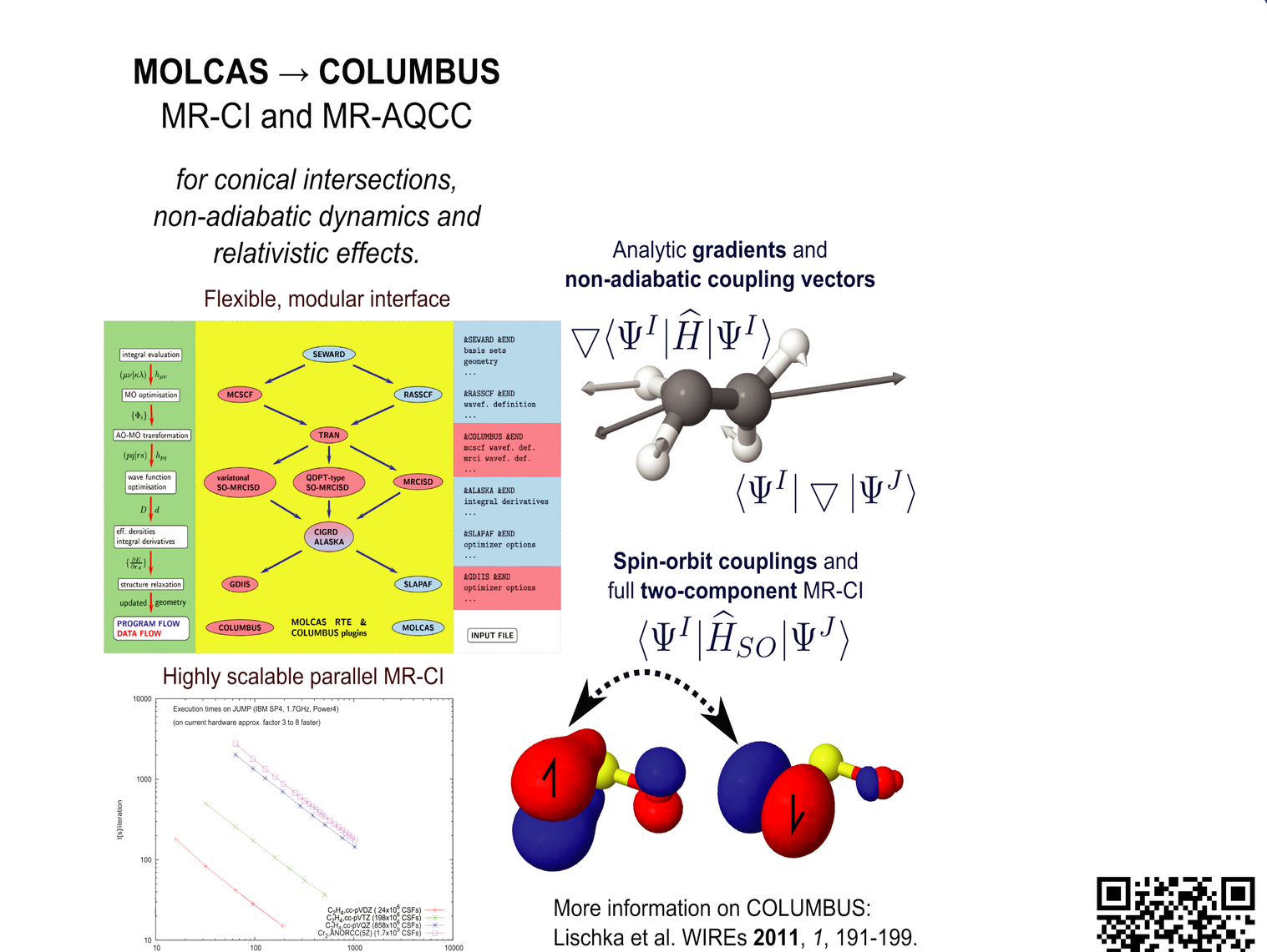


P.O.Widmark, V.Vysotskiy, T.Tsuchiya, V.Veryazov

Parallel CASPT2

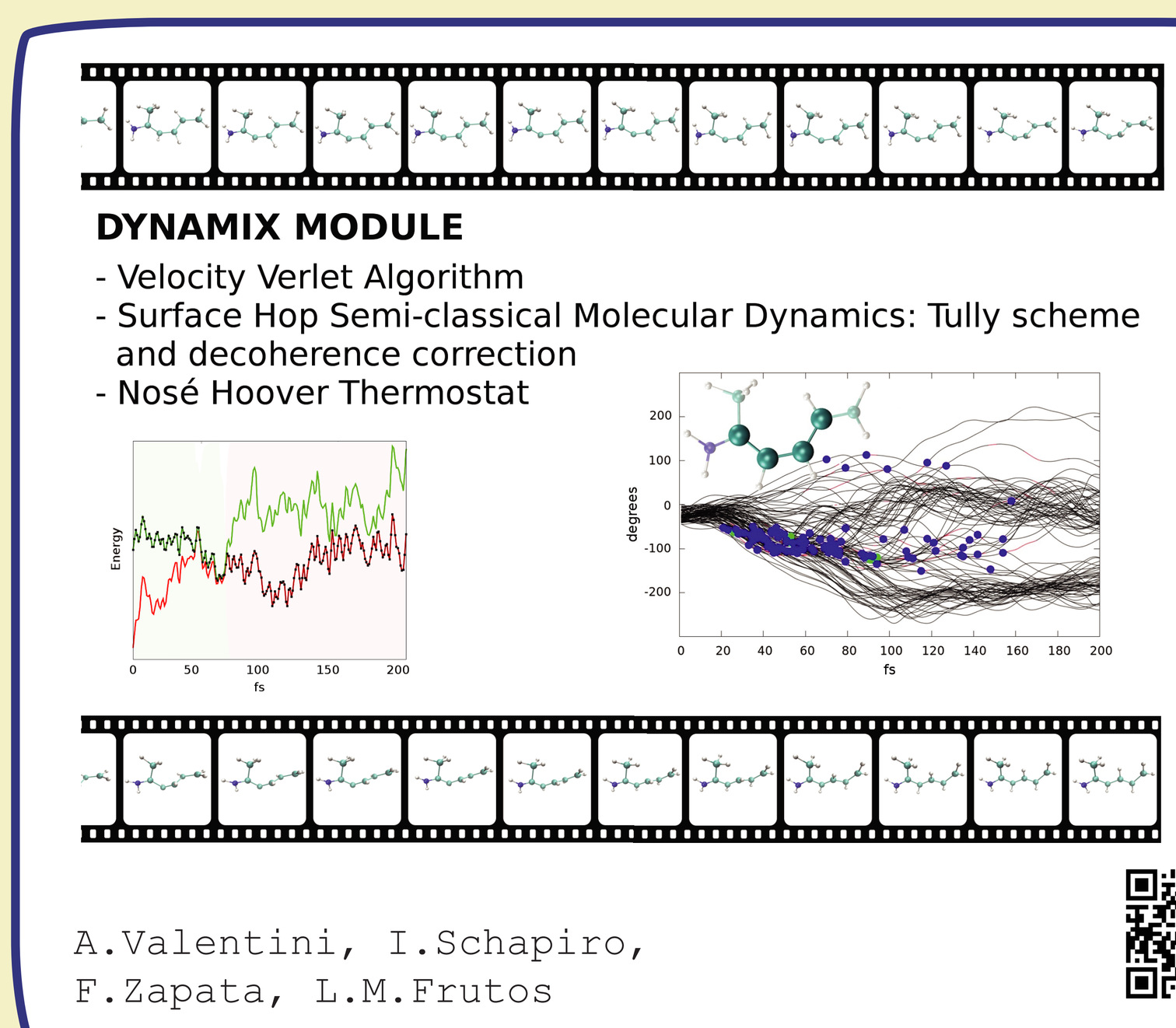


S.Vancoillie,V.Vysotskiy,P.Å.Malmqvist



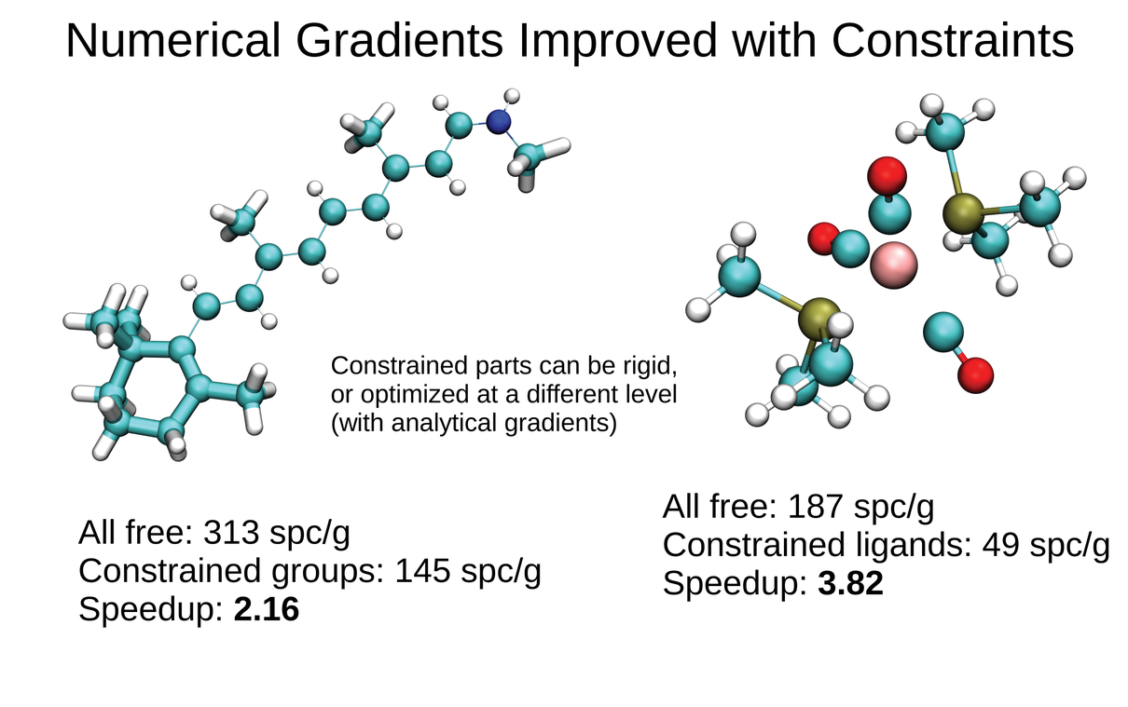
MOLCAS → COLUMBUS
MR-CI and MR-AQCC
for conical intersections, non-adiabatic dynamics and relativistic effects.
Flexible, modular interface
Analytic gradients and non-adiabatic coupling vectors
Spin-orbit couplings and full two-component MR-CI
Highly scalable parallel MR-CI
More information on COLUMBUS: Lischka et al. WIREs 2011, 1, 191-199.

H.Lischka, T.Mueller, F.Plasser



A.Valentini, I.Schapiro, F.Zapata, L.M.Frutos

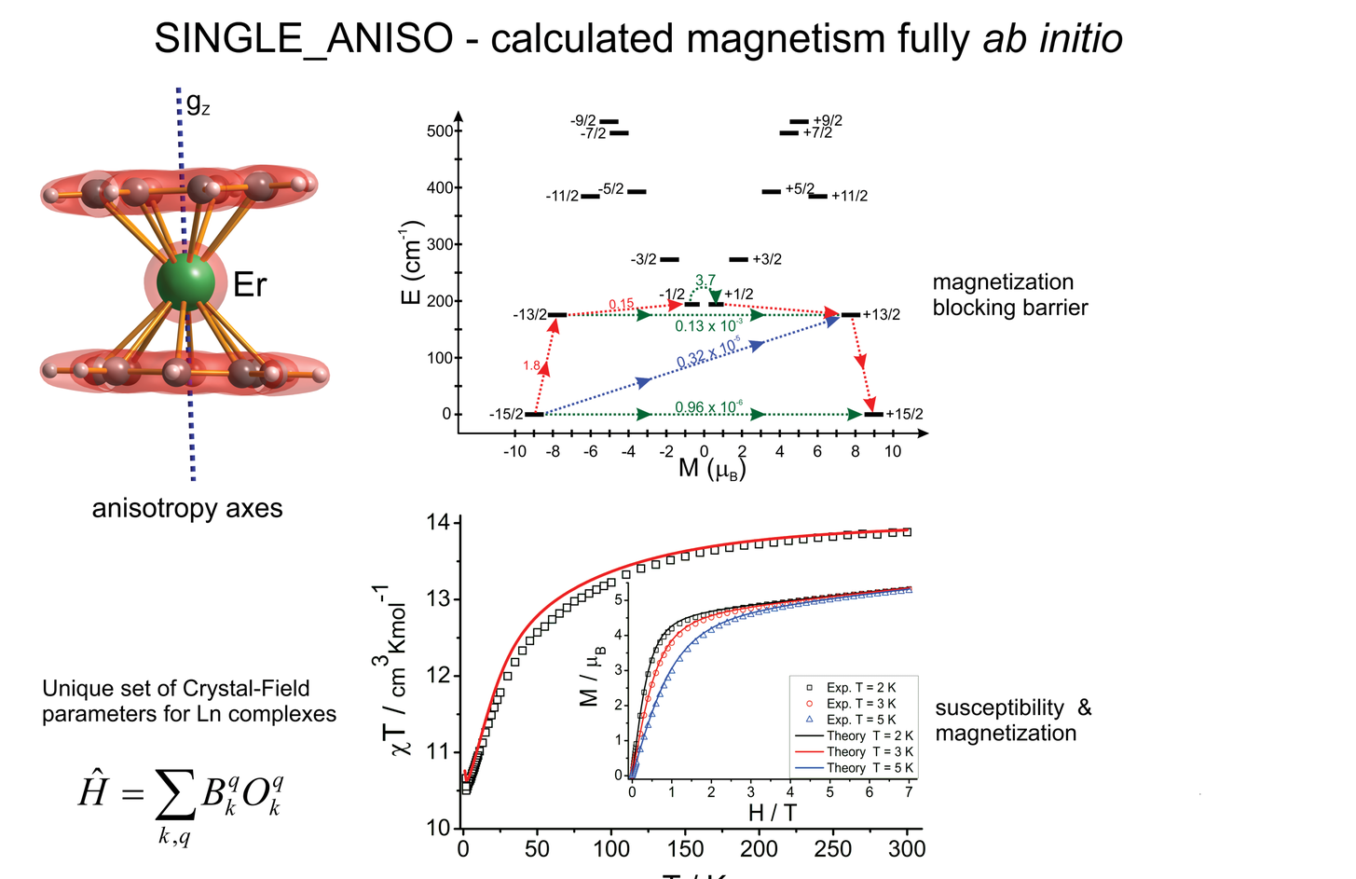
Numerical Gradients Improved with Constraints



spc/g = single-point calculations per gradient

I.Fernández Galván, R.Lindh

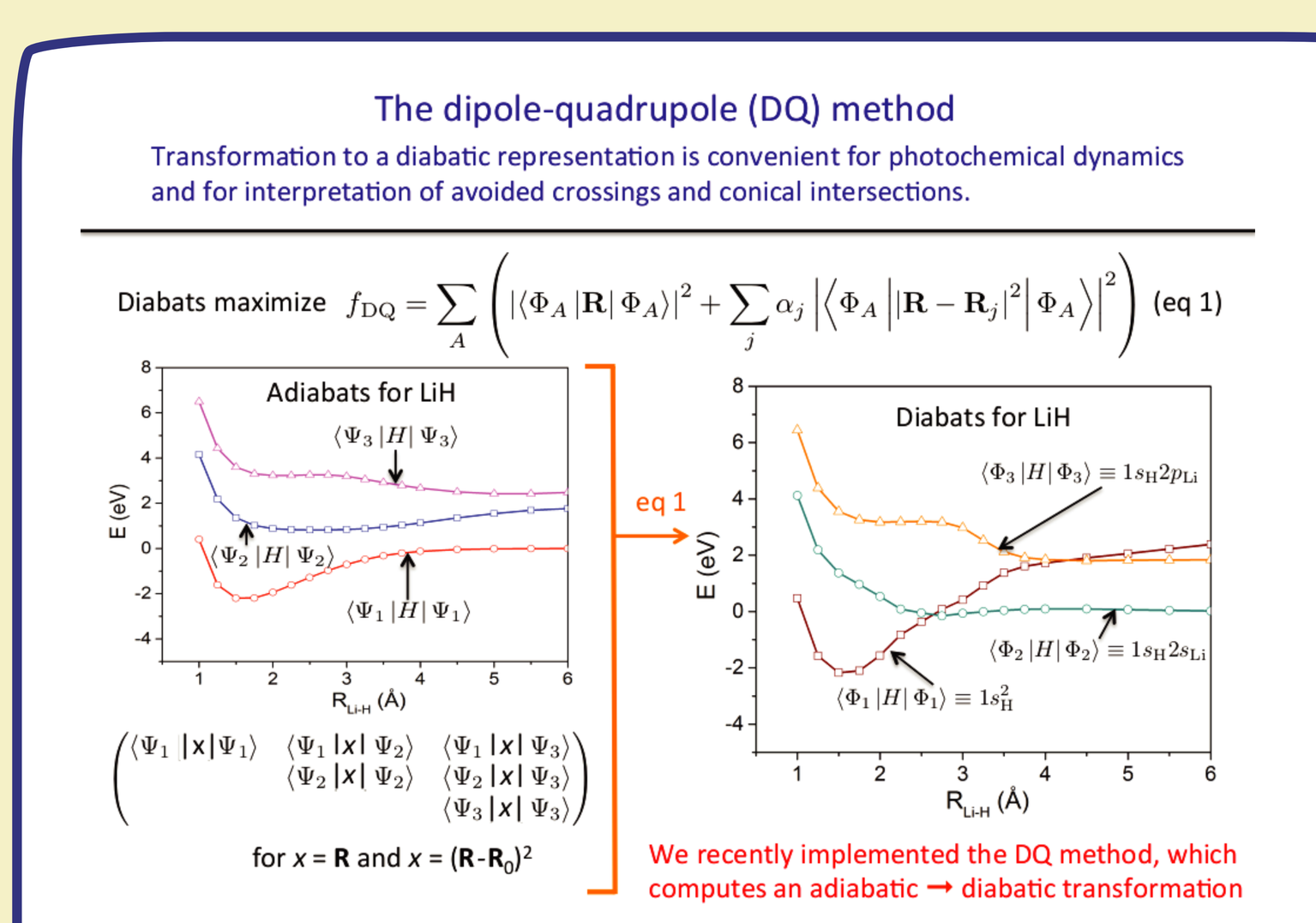
SINGLE_ANISO - calculated magnetism fully *ab initio*



L.F.Chibotaru, L.Ungur

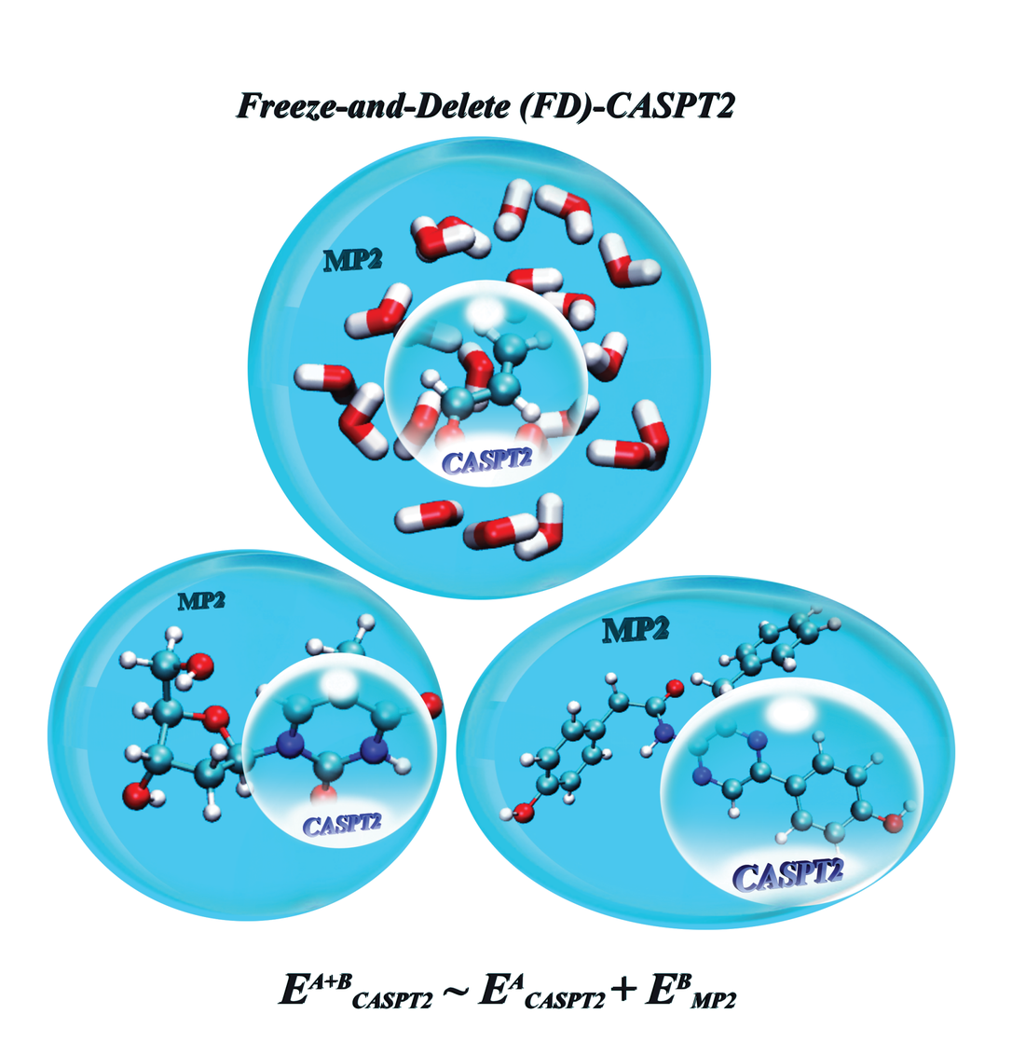
The dipole-quadrupole (DQ) method

Transformation to a diabatic representation is convenient for photochemical dynamics and for interpretation of avoided crossings and conical intersections.



C.E.Hoyer, X.Xu, D.Ma, L.Gagliardi, D.G.Truhlar

Freeze-and-Delete (FD)-CASPT2

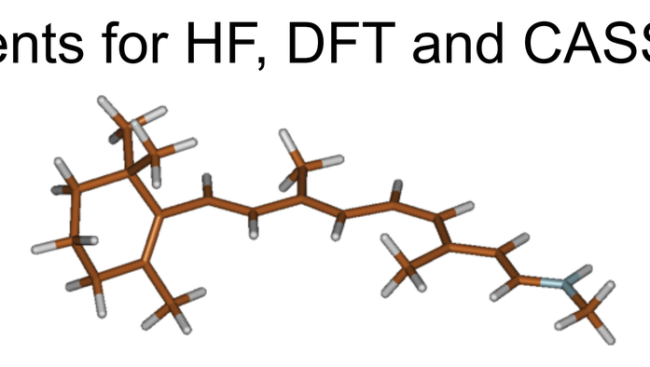


$E^{A+B}_{CASPT2} \sim E^{A}_{CASPT2} + E^{B}_{MP2}$

F.Aquilante, P.Farahani

Coming soon..

RI gradients for HF, DFT and CASSCF



Retinal ANO-S-VDZP : 54 atoms (22 non-H atoms), 468 bsf, CAS (12,12)

	State-specific		State-averaged	
	Conventional	RICD	Conventional	RICD
Energy	15h04	1h09 (7.6%)	15h41	1h49 (11.6%)
Gradient	9h20	47m (8.4%)	> 150h	8h36 (<6%)
Total	24h24	1h56 (7.9%)	> 168h	10h25 (<6%)

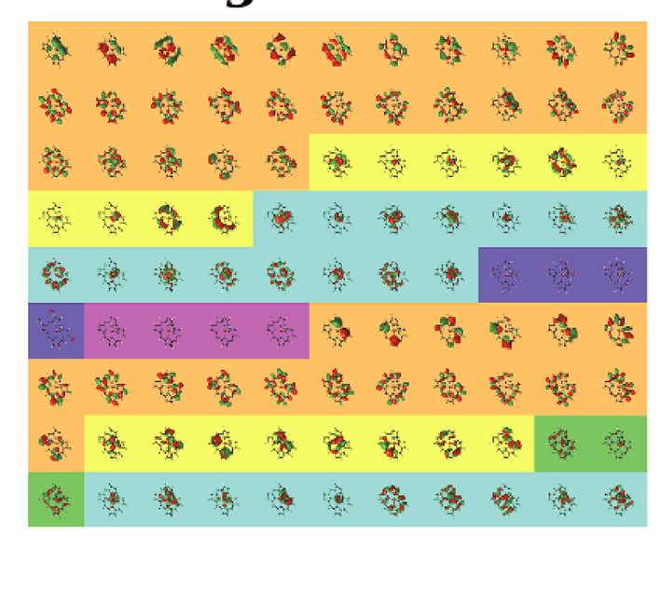
M.Delcey, R.Lindh

DMRG-SCF+PT2 and gradients

Active space limitations:

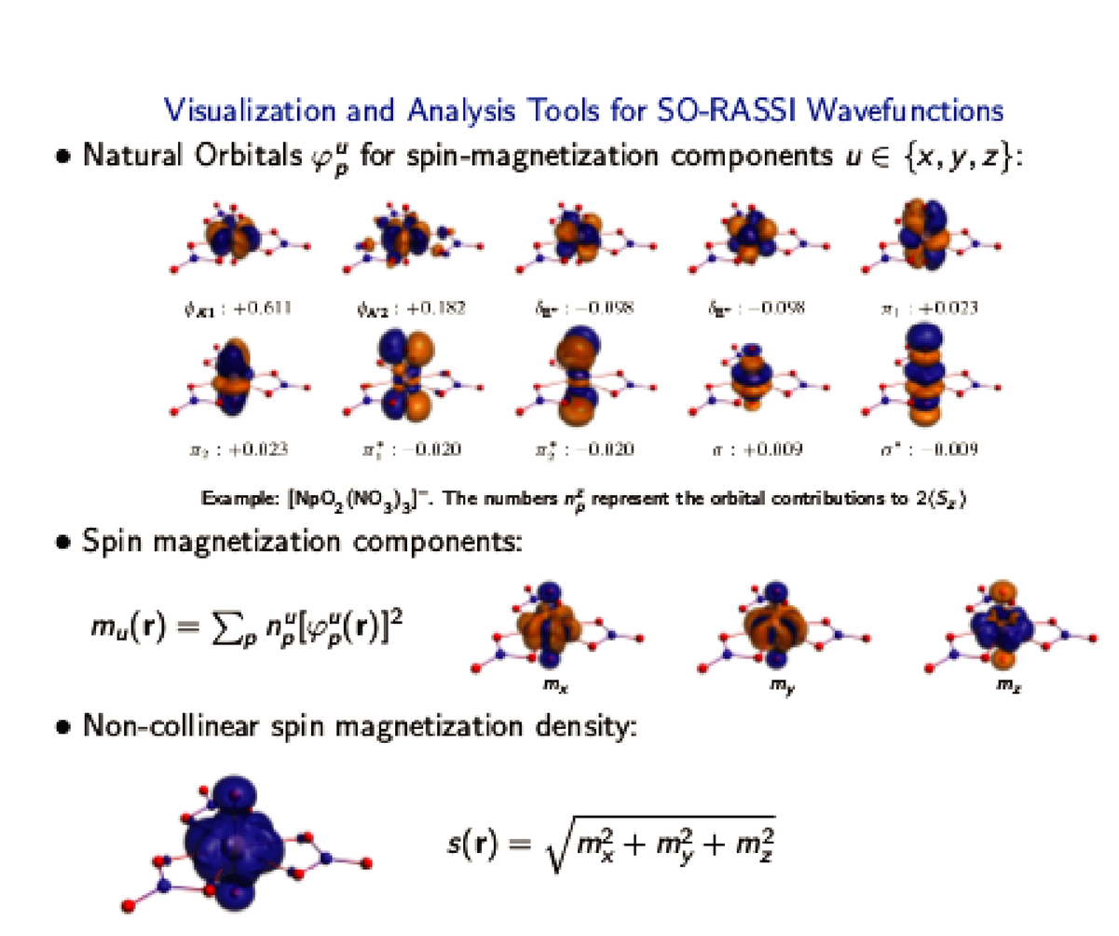
CAS - 16

RAS - 32



QC-MAQUIS(DMRG)>> 50

S.Keller, Y.Ma, S.Knecht, M.Reiher



J.Autschbach

Supported platforms

AIX · INFINIBAND TRADE ASSOCIATION CERTIFIED · IBM Blue Gene · CRAY XE6

http://www.molcas.org