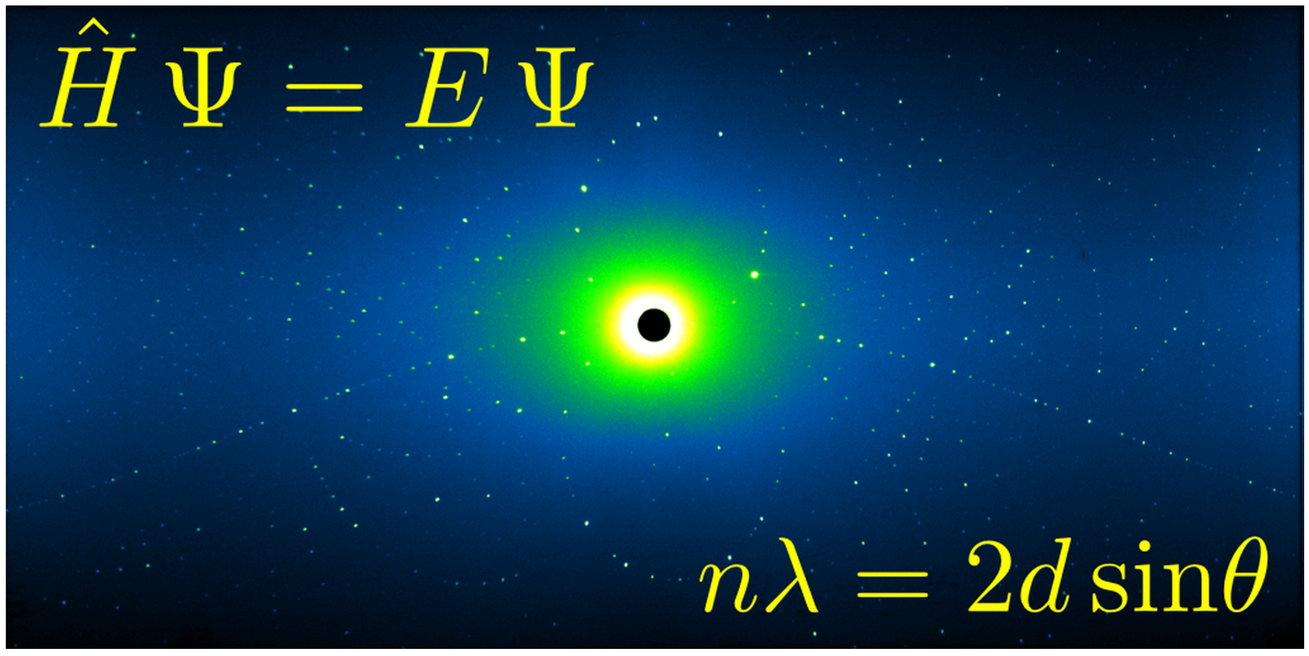
Alessandro Genoni
CNRS & Université de Lorraine, Laboratoire LPCT, Metz, France

About the Connections and Possible Contaminations between Quantum Chemistry and Quantum Crystallography



3rd Quantum International Frontier - QIF3
Łódź, Poland - June 24, 2023

Goal of the Pedagogical Lecture and Historical Background

Showing (and possibly inspiring) possible connections between Quantum Chemistry and Crystallography
(and particularly between Quantum Chemistry and Quantum Crystallography)

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Initial connections in the early days of Quantum Physics,
which were contemporary of the transformation from the old to the modern crystallography

Early quantum physicists soon realized that high-energy radiations could be also exploited to “visualize”
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> *"It seems to me that the experimental study of scattered radiation, in particular from light atoms, should get more attention, since along this way it should be possible to determine the arrangement of the electrons in the atoms"*

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"It is hoped that it will be possible in this manner [through X-ray diffraction] to obtain more definite information concerning the distribution of electrons in the atoms"

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Quantum Crystallography Today

Previous words by Debye and Compton ⟶ Starting point of Quantum Crystallography

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- multipole model techniques for the determination of experimental charge and spin densities (e.g., Hansen & Coppens model)
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X-ray structure factors are Fourier transforms of the (unit-cell) electron density:

$$F_{\mathbf{h}} = \int_{cell} d\mathbf{r}\ \rho(\mathbf{r})\ e^{i2\pi\mathbf{r}\cdot(\mathbf{Bh})}$$

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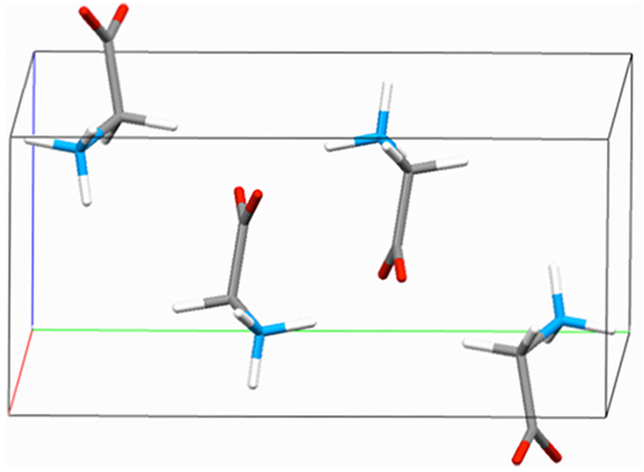
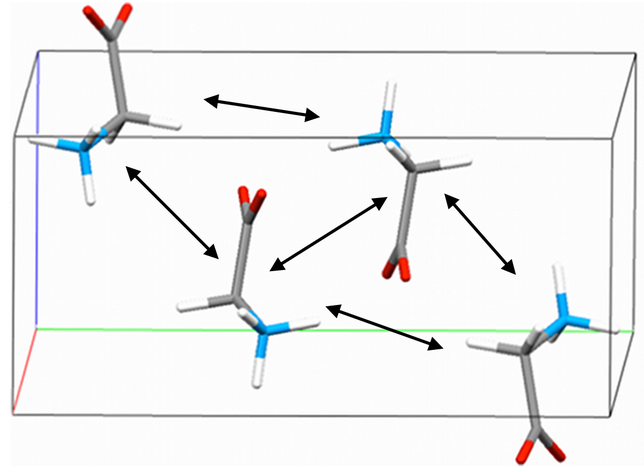
    a. each crystal-unit does not interact with the other ones

Fictitious Non-Interacting Crystal



VS

Real Interacting Crystal



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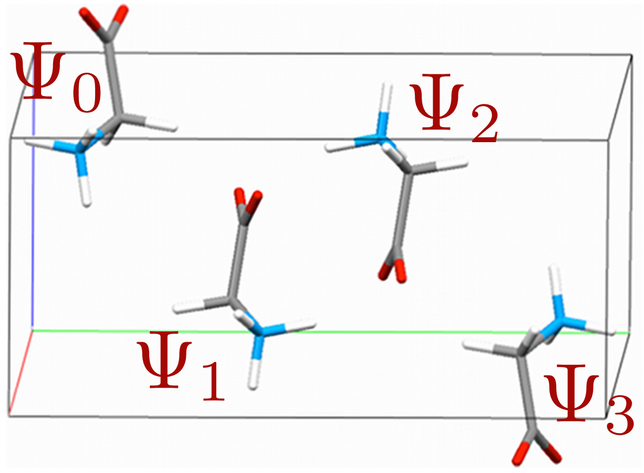
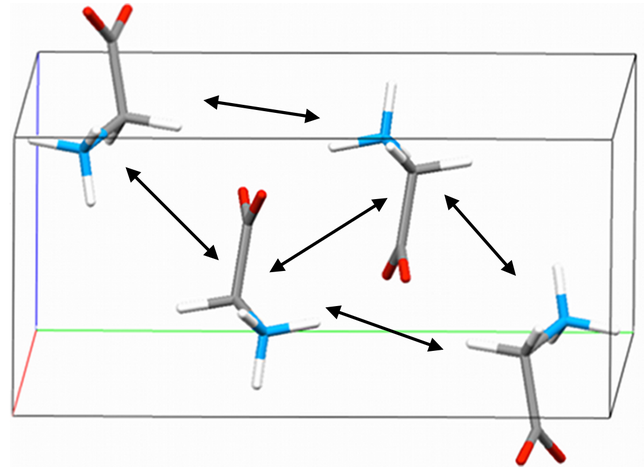


$$\rho^{F}_{cell}(\mathbf{r}) = \rho_{cell}(\mathbf{r})$$

Real Interacting Crystal



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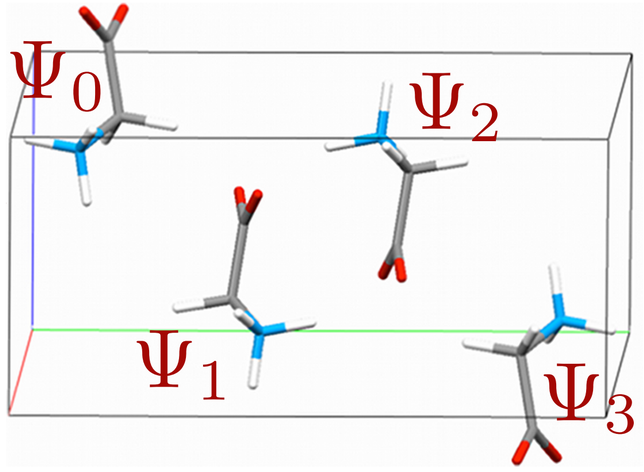
3. Each crystal-unit wavefunction has a well-defined form according to the chosen *ansatz* (e.g., single Slater determinant)

Fictitious Non-Interacting Crystal



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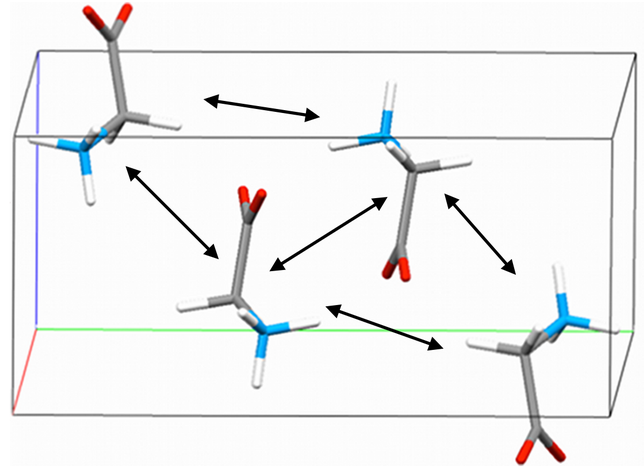

X-ray Restrained Wavefunction: Basic Assumptions (2)

The unit-cell electron density for the fictitious crystal can be written as

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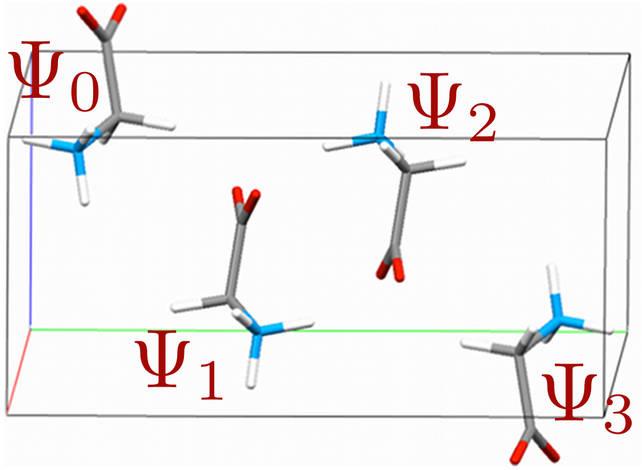

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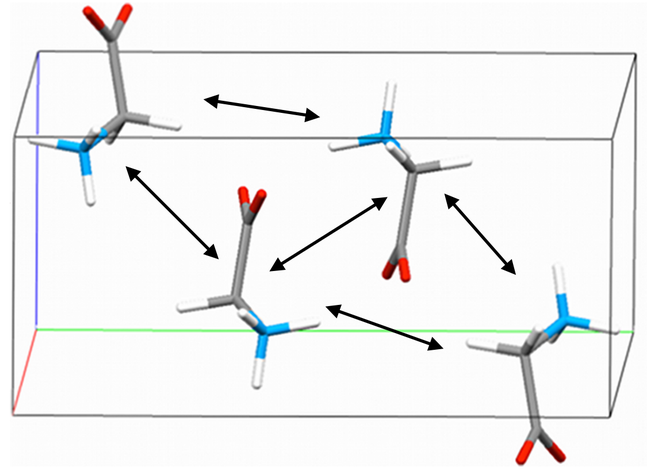

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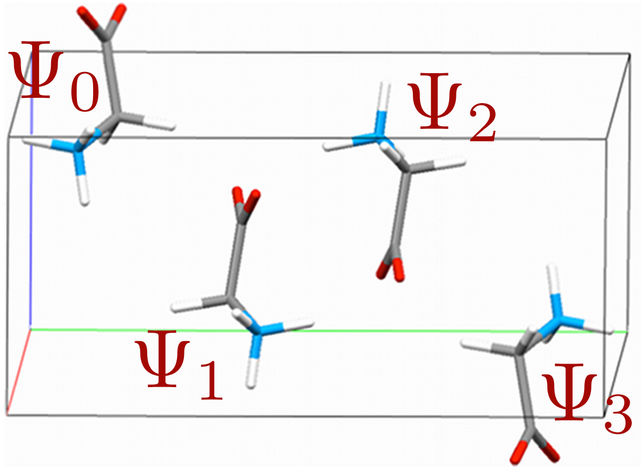

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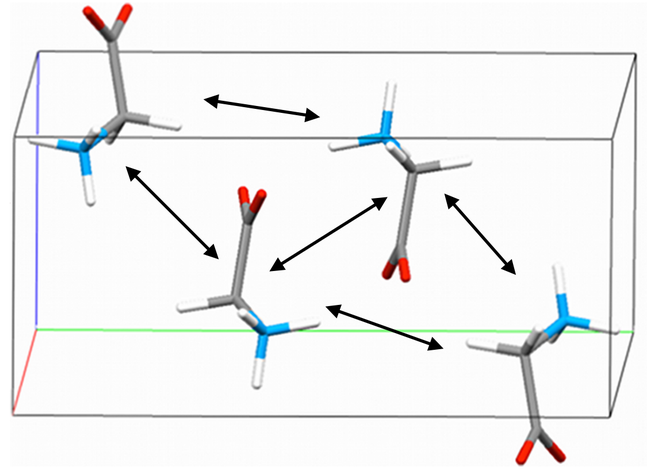

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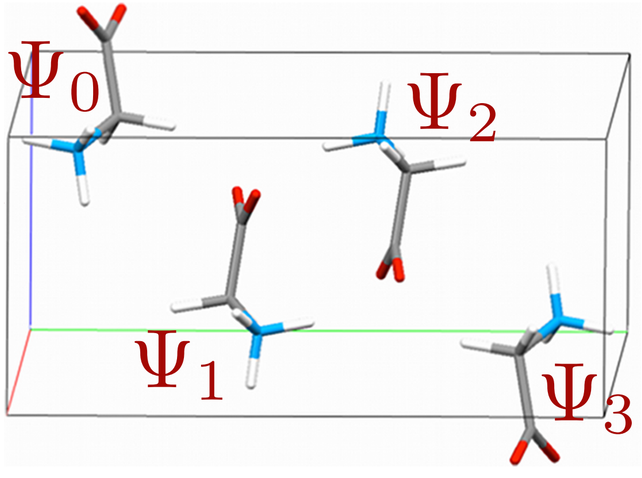

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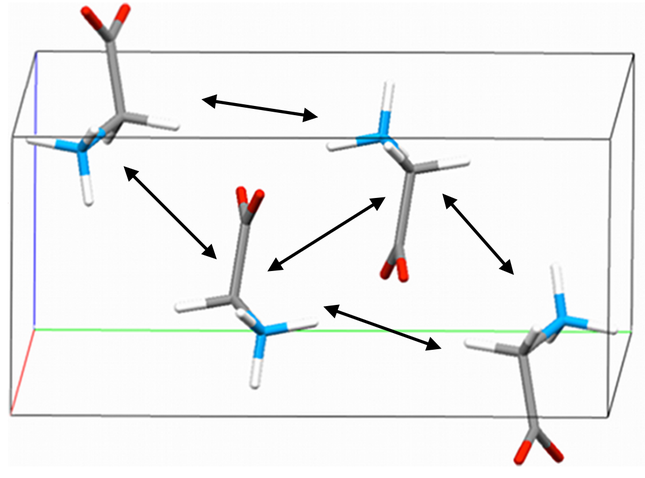

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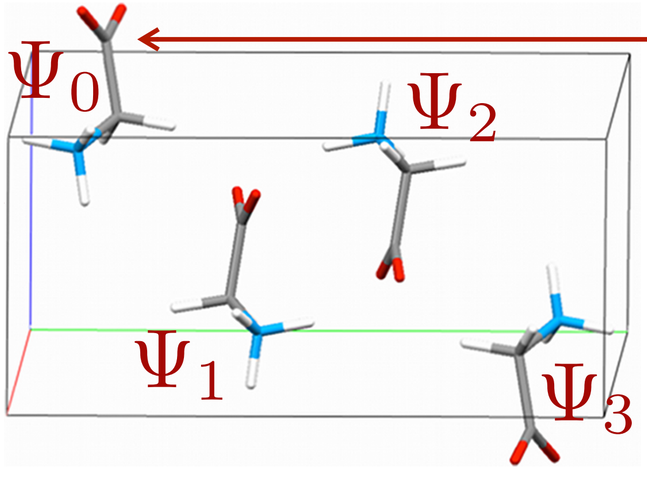

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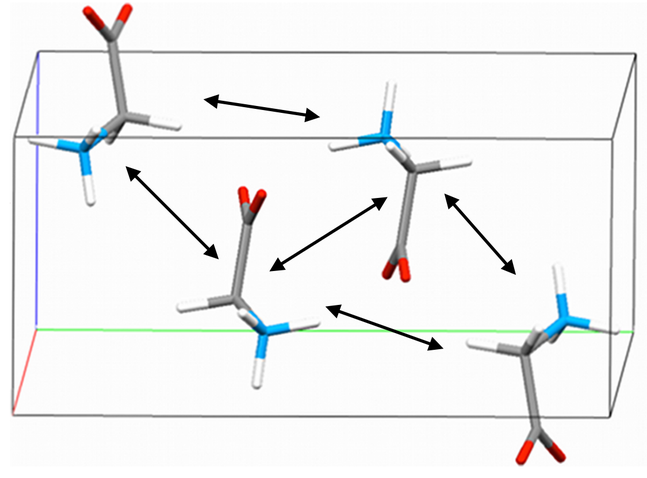

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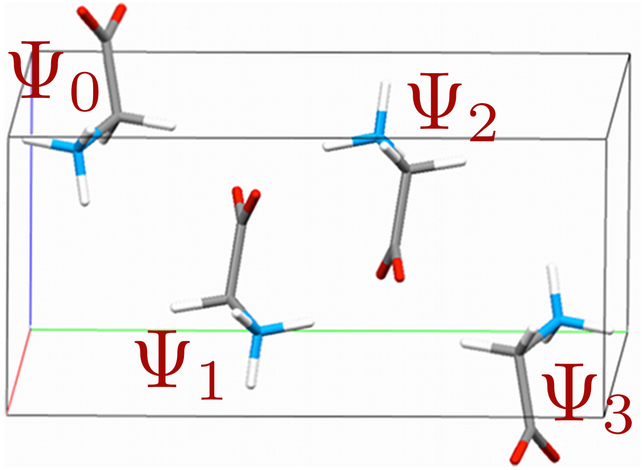

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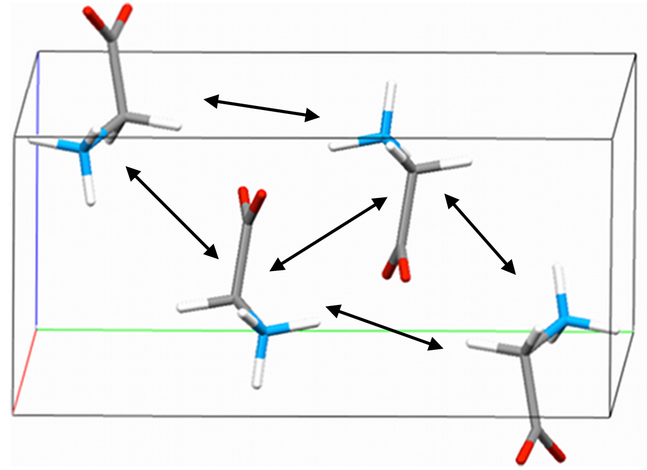

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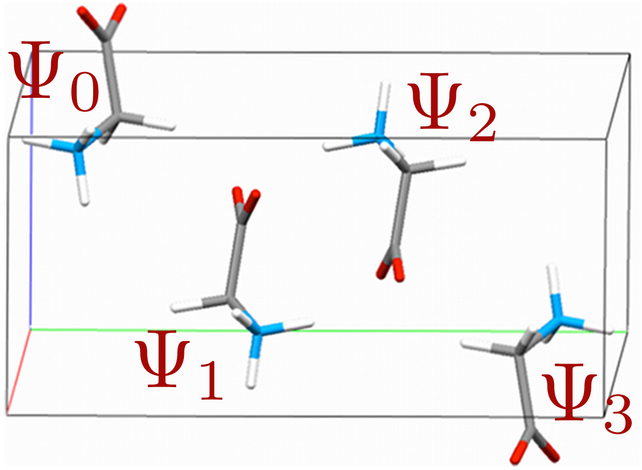

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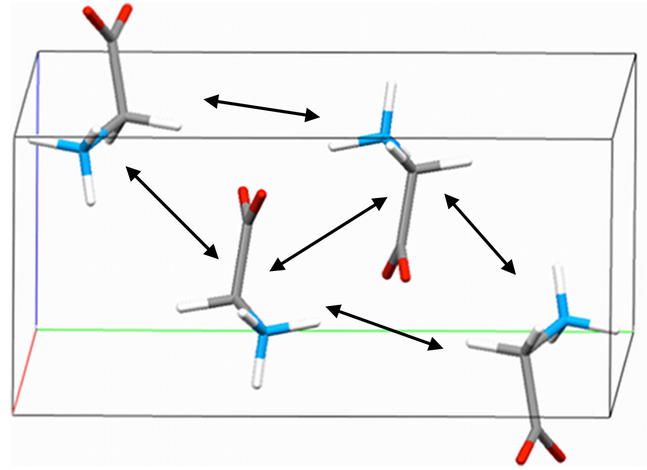

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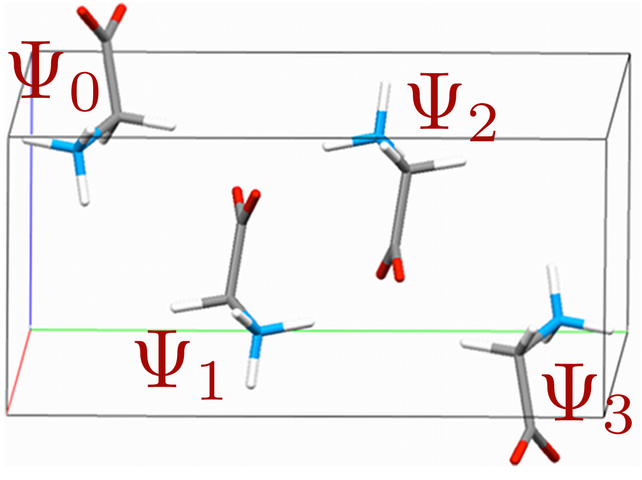

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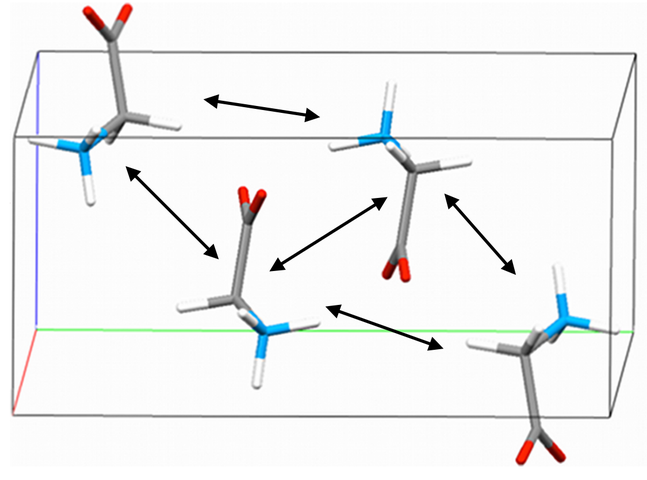

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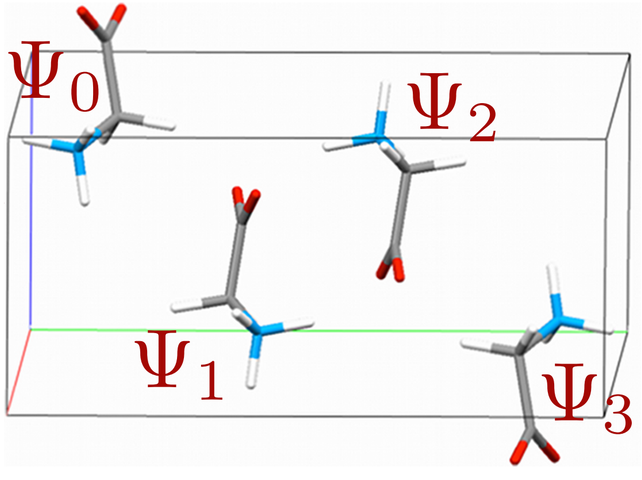

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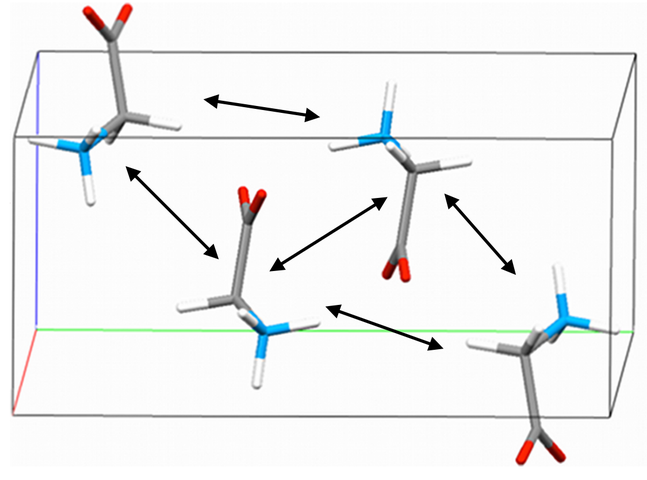

X-ray Restrained Wavefunction Method: the Eigenvalue Equation

Equivalent to finding those MOs that minimize this functional:

$$J[\Psi] = \langle \Psi | \hat{H} | \Psi \rangle + \lambda \, \chi^2$$

D. Jayatilaka, *Phys. Rev. Lett.* **80**, 798 (1998)

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Measure of the statistical agreement:

$$\chi^2[\Psi] = \frac{1}{N_r - N_p} \sum_{\mathbf{h}} \frac{\left(\eta \left| F_{\mathbf{h}}^{calc} \right| - \left| F_{\mathbf{h}}^{exp} \right| \right)^2}{\sigma_{\mathbf{h}}^2}$$

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Equivalent to finding those MOs that minimize this functional:

$$J[\Psi] = \langle \Psi | \hat{H} | \Psi \rangle + \lambda \, \chi^2$$

External multiplier gradually and manually adjusted during the calculations

Measure of the statistical agreement:

$$\chi^2[\Psi] = \frac{1}{N_r - N_p} \sum_{\mathbf{h}} \frac{\left(\eta \left| F_{\mathbf{h}}^{calc} \right| - \left| F_{\mathbf{h}}^{exp} \right| \right)^2}{\sigma_{\mathbf{h}}^2}$$

THE NEW EIGENVALUE EQUATION:

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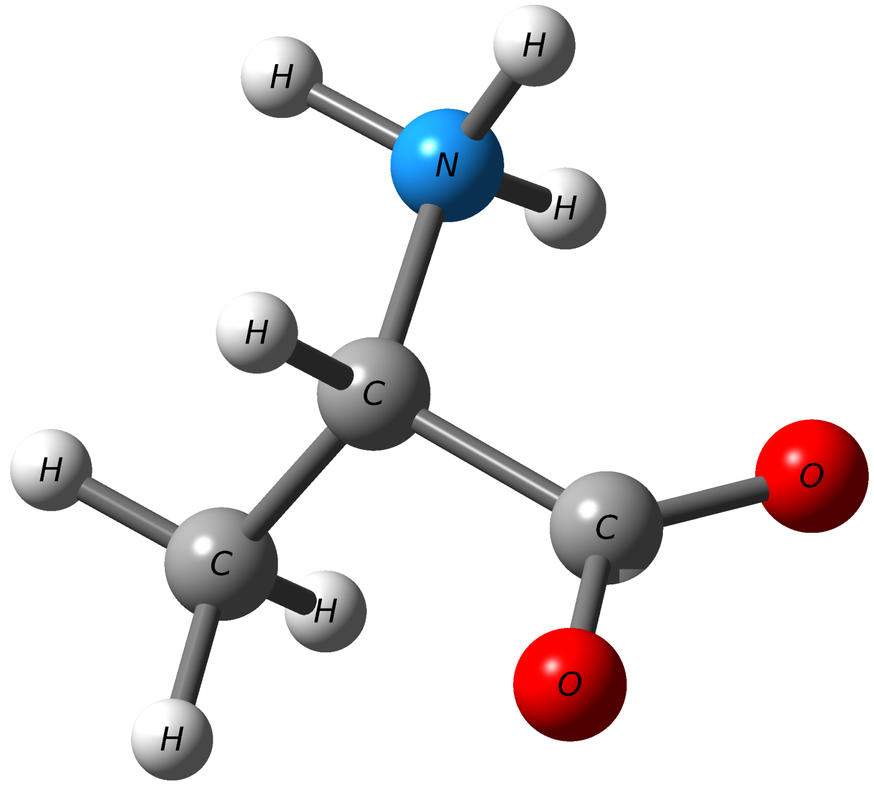
X-ray Restrained Wavefunction Calculations: An Example (1)

- L-alanine crystal structure determined at 23 K.

- Single-point calculations (crystal geometry) at Hartree-Fock, B3LYP and XR-Hartree-Fock levels with basis sets of increasing size and flexibility:
  * 3-21G
  * 6-31G(d)
  * cc-pVDZ
  * 6-311G(d,p)
  * aug-cc-pVDZ
  * 6-311++G(2d,2p)

- X-ray restrained wavefunction calculations with unit-cell parameters, thermal parameters and structure factor amplitudes deposited with the crystal structure.



R. Destro *et al.*, *J. Phys. Chem.* **92**, 966 (1988)

X-ray Restrained Wavefunction Calculations: An Example (2)

VALUES OF THE STATISTICAL AGREEMENTS (χ^2)

Basis-Set	RHF	B3LYP	XR-RHF (λ_{max})
3-21G	5.66	3.70	1.71 (0.58)
6-31G(d)	2.94	2.18	1.26 (0.32)
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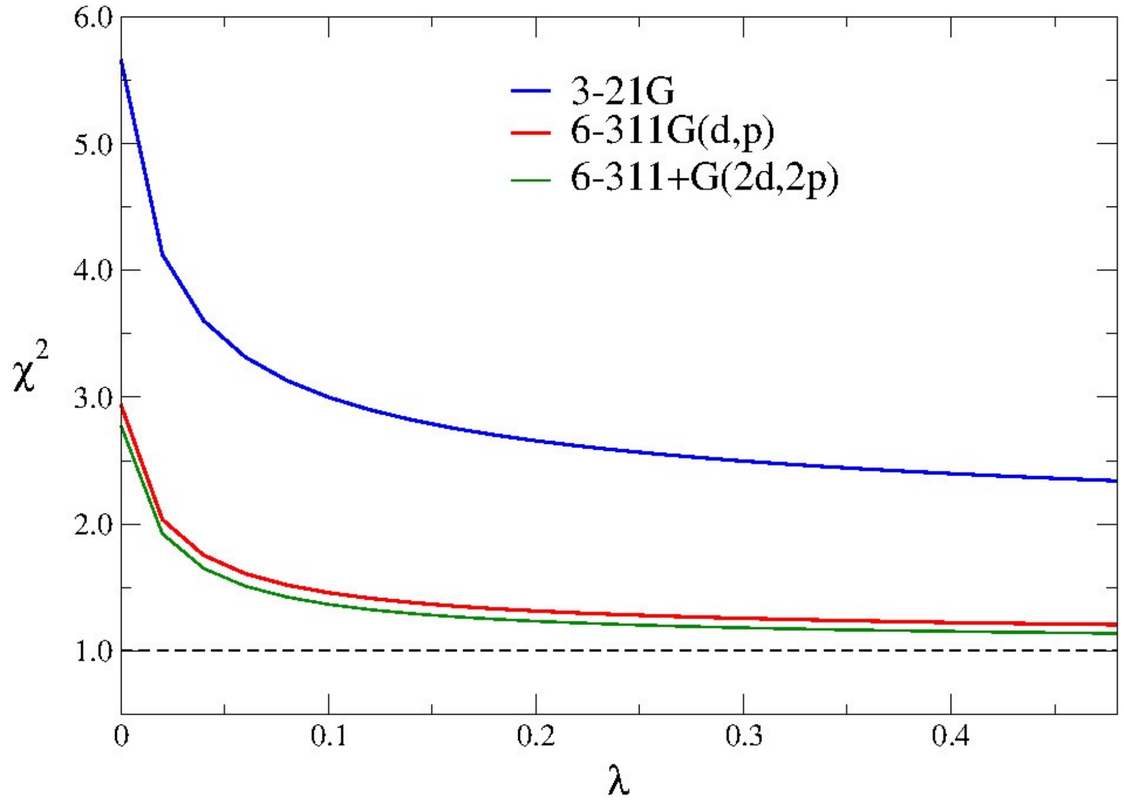

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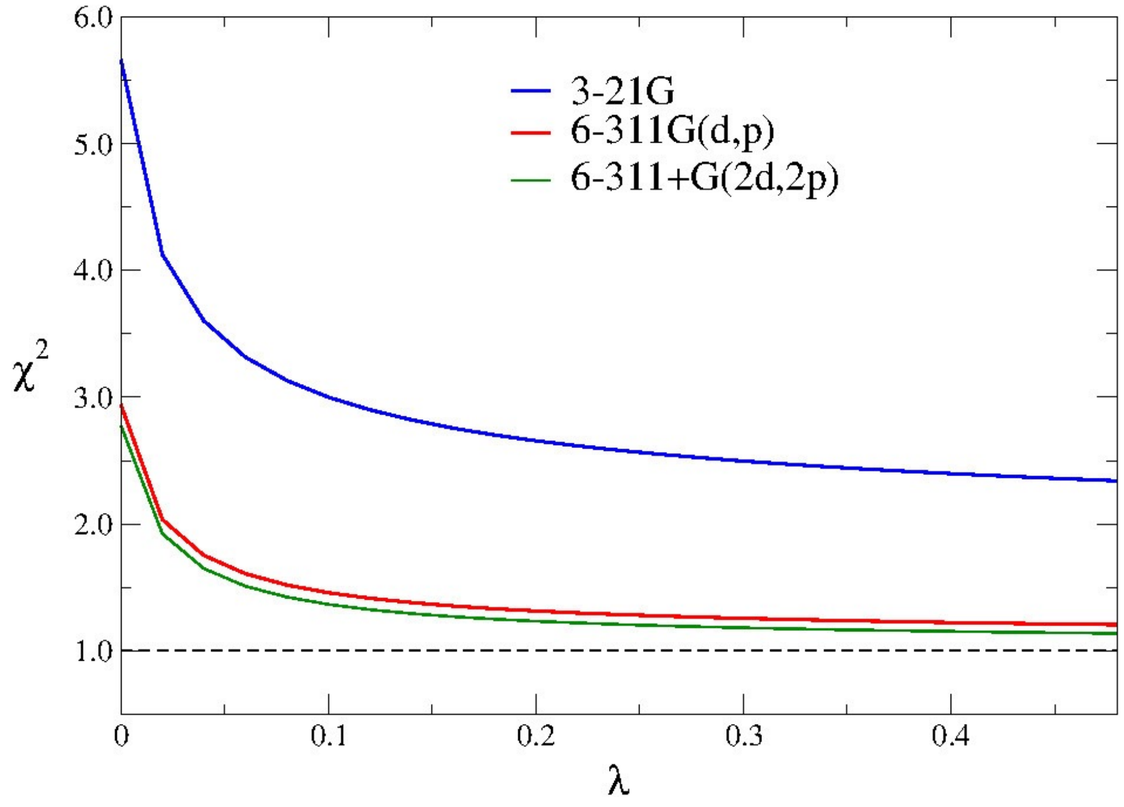

IF GOOD-QUALITY CRYSTALLOGRAPHIC DATA ARE AVAILABLE AND SUFFICIENTLY FLEXIBLE BASIS-SETS ARE USED, THE IDEAL STATISTICAL AGREEMENT CAN BE REACHED QUITE EASILY

Correlation and Crystal Field Effects in X-ray Data

X-ray structure factors are Fourier transforms of the (unit-cell) electron density $\longrightarrow$ $F_{\mathbf{h}} = \int_{cell} d\mathbf{r}\ \rho(\mathbf{r})\ e^{i2\pi\mathbf{r}\cdot(\mathbf{Bh})}$

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X-ray structure factors should intrinsically contain electron correlation and crystal-field effects on the electron density

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4. X-ray structure factors from single-molecule X-ray diffraction experiments (e.g., X-ray free electron laser experiments)
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IUCrJ
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Can X-ray constrained Hartree–Fock wavefunctions retrieve electron correlation?

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The Journal of Chemical Physics ARTICLE scitation.org/journal/jcp

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Let us see a preliminary attempt…

XRW Equations as Generalized Kohn-Sham Equations

Let us rewrite the XRW equations for a *2N*-electron closed-shell system as follows:

$$\hat{F}^{xrw}\ \phi_i^{xrw}(\mathbf{r}) = \left[-\frac{1}{2}\nabla^2 + v(\mathbf{r}) + 2\,\hat{G} + \hat{K} + \hat{v}^{xrw}\right]\ \phi_i^{xrw}(\mathbf{r}) = \epsilon_i^{xrw}\ \phi_i^{xrw}(\mathbf{r})$$

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- $\hat{v}^{xrw}$ as the Jayatilaka operator due to the perturbation of the X-ray data used as restraints

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The XRW equations can be rewritten in the form of generalized Kohn-Sham equations (with exact exchange):

$$\left[-\frac{1}{2}\nabla^2 + v(\mathbf{r}) + v_H(\mathbf{r}) + \hat{u}_{xc}^{xrw}\right]\ \phi_i^{xrw}(\mathbf{r}) = \epsilon_i^{xrw}\ \phi_i^{xrw}(\mathbf{r})$$

$$\hat{u}_{xc}^{xrw} = \hat{K} + \hat{v}^{xrw}$$

XRW Equations as Generalized Kohn-Sham Equations

Let us rewrite the XRW equations for a *2N*-electron closed-shell system as follows:

$$\hat{F}^{xrw}\ \phi_i^{xrw}(\mathbf{r}) = \left[-\frac{1}{2}\nabla^2 + v(\mathbf{r}) + 2\,\hat{G} + \hat{K} + \hat{v}^{xrw}\right]\ \phi_i^{xrw}(\mathbf{r}) = \epsilon_i^{xrw}\ \phi_i^{xrw}(\mathbf{r})$$

- $v(\mathbf{r})$ as the external potential
- $\hat{G}$ and $\hat{K}$ as the Coulomb and Exchange operators
- $\hat{v}^{xrw}$ as the Jayatilaka operator due to the perturbation of the X-ray data used as restraints

$$\hat{v}^{xrw} = \lambda \sum_{\mathbf{h}} K_{\mathbf{h}}\,\mathrm{Re}\{F_{\mathbf{h}}^{calc}\}\,\hat{I}_{\mathbf{h},R} + \lambda \sum_{\mathbf{h}} K_{\mathbf{h}}\,\mathrm{Im}\{F_{\mathbf{h}}^{calc}\}\,\hat{I}_{\mathbf{h},C} \quad \text{with} \quad K_{\mathbf{h}} = \frac{2\eta}{N_r - N_p}\,\frac{\eta\left|F_{\mathbf{h}}^{calc}\right| - \left|F_{\mathbf{h}}^{exp}\right|}{\sigma_{\mathbf{h}}^2\left|F_{\mathbf{h}}^{calc}\right|}$$

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$$\hat{u}_{xc}^{xrw} = \hat{K} + \hat{v}^{xrw}$$

These generalized Kohn-Sham equations can be inverted to obtain the corresponding XRW exchange-correlation potentials (associated with the X-ray diffraction data)

Orbital-Averaged XRW Exchange-Correlation Potentials (1)

$$\left[-\frac{1}{2}\nabla^2 + v(\mathbf{r}) + v_H(\mathbf{r}) + \hat{u}_{xc}^{xrw}\right]\ \phi_i^{xrw}(\mathbf{r}) = \epsilon_i^{xrw}\ \phi_i^{xrw}(\mathbf{r})$$

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- multiplying the equation by $2\,\phi_i^{xrw*}(\mathbf{r})$ (to be done for each occupied molecular orbital)
- summing the results of the previous multiplications, over i from 1 to N
- dividing by the XRW electron density $\rho^{XRW}(\mathbf{r})$

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→ XRW inversion formula (analogous to the Kohn-Sham inversion formula)

$$\overline{v_{xc}^{xrw}}(\mathbf{r}) = \overline{\epsilon^{xrw}}(\mathbf{r}) - \frac{\tau^{xrw}(\mathbf{r})}{\rho^{xrw}(\mathbf{r})} + \frac{1}{4}\,\frac{\nabla^2\rho^{xrw}(\mathbf{r})}{\rho^{xrw}(\mathbf{r})} - v(\mathbf{r}) - v_H(\mathbf{r})$$

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where:

$$\overline{v_{xc}^{xrw}}(\mathbf{r}) = \frac{2}{\rho^{xrw}(\mathbf{r})}\sum_{i=1}^{N}\ \phi_i^{xrw*}(\mathbf{r})\ \hat{u}_{xc}^{xrw}\ \phi_i^{xrw}(\mathbf{r}) \longrightarrow$$ **orbital-averaged** XRW exchange-correlation potential

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$$\overline{\epsilon^{xrw}}(\mathbf{r}) = \frac{2}{\rho^{xrw}(\mathbf{r})}\sum_{i=1}^{N}\ \epsilon_i^{xrw}\ |\phi_i^{xrw}(\mathbf{r})|^2 \longrightarrow \text{average local XRW orbital energy}$$

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$$\tau^{xrw}(\mathbf{r}) = \sum_{i=1}^{N}\left|\nabla\phi_i^{xrw}(\mathbf{r})\right|^2 \longrightarrow \text{positive-definite form of the XRW kinetic energy density}$$

Orbital-Averaged XRW Exchange-Correlation Potentials (2)

$$\overline{v_{xc}^{xrw}}(\mathbf{r}) = \overline{\epsilon^{xrw}}(\mathbf{r}) - \frac{\tau^{xrw}(\mathbf{r})}{\rho^{xrw}(\mathbf{r})} + \frac{1}{4}\,\frac{\nabla^2\rho^{xrw}(\mathbf{r})}{\rho^{xrw}(\mathbf{r})} - v(\mathbf{r}) - v_H(\mathbf{r})$$

An **orbital-averaged XRW exchange-correlation potential** can be simply obtained from an external potential $v(\mathbf{r})$, a given set of occupied X-ray restrained molecular orbitals $\left\{\phi_i^{xrw}(\mathbf{r})\right\}$, and a given set of X-ray restrained orbital energies $\left\{\epsilon_i^{xrw}\right\}$

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Possibility of determining orbital-averaged XRW "correlation"potentials:

$$\overline{v_c^{xrw}}(\mathbf{r}) = \overline{v_{xc}^{xrw}}(\mathbf{r}) - \overline{v_x^{xrw}}(\mathbf{r})$$

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→ both potentials constructed using the same density

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$\overline{v_{xc}^{xrw}}(\mathbf{r})$ → orbital-averaged XRW exchange-correlation potential (seen above)

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In particular:

$\overline{v_{xc}^{xrw}}(\mathbf{r})$ → orbital-averaged XRW exchange-correlation potential (seen above)

$\overline{v_x^{xrw}}(\mathbf{r})$ → obtained by exploiting the inversion formula with molecular orbitals and orbital energies resulting from the simple diagonalization of the exchange-only Kohn-Sham Hamiltonian constructed with the self-consistent XRW molecular orbitals

Some Caveats about the Orbital-Averaged XRW Potentials…

The presented strategy is a density-to-potential mapping

↓

Fitting of the exchange-correlation potential to the target density

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   [see Kananenka *et al.*, *J. Chem. Phys.* **139**, 074112 (2013); Gaiduk *et al.*, *J. Chem Theory Comput.* **9**, 3959 (2013)]

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↓

Extraction of $v_{xc}^{xrw}(\mathbf{r})$ and $v_{c}^{xrw}(\mathbf{r})$ potentials from X-ray data by going beyond the inversion of the XRW equations
(e.g., by exploiting the modified Ryabinkin-Kohut-Staroverov approach)

Neon: CCSD/UGBS Gas-Phase X-ray Structure Factors

Type of X-ray structure factors: gas-phase theoretically generated

Level of theory / basis set: CCSD / UGBS

Size of the fictitious cubic unit-cell: 10.0 $\mathrm{\AA}$

Limit of structure factor resolution: 2.0 $\mathrm{\AA}^{-1}$ (namely, 0.25 $\mathrm{\AA}$)

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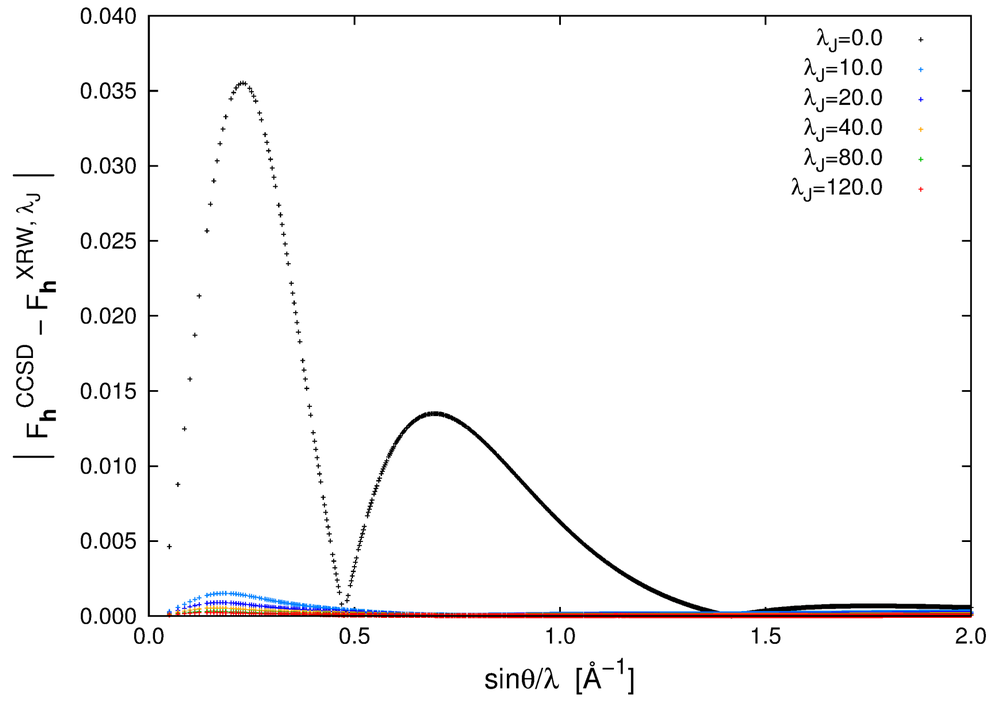

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0.0	0.1194
10.0	0.0044
40.0	0.0015
80.0	0.0010
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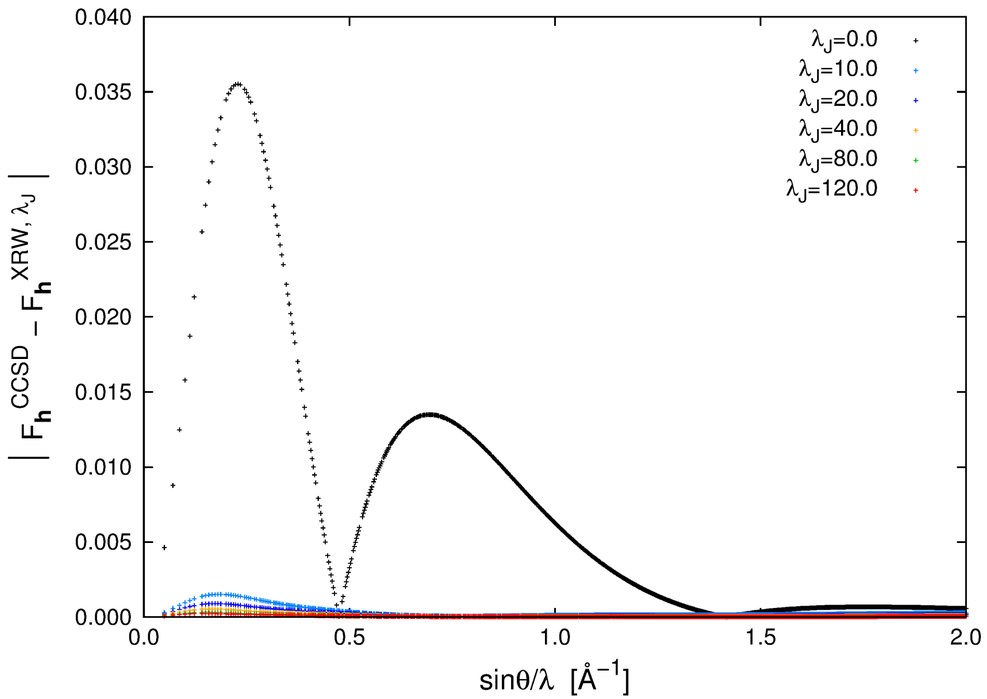

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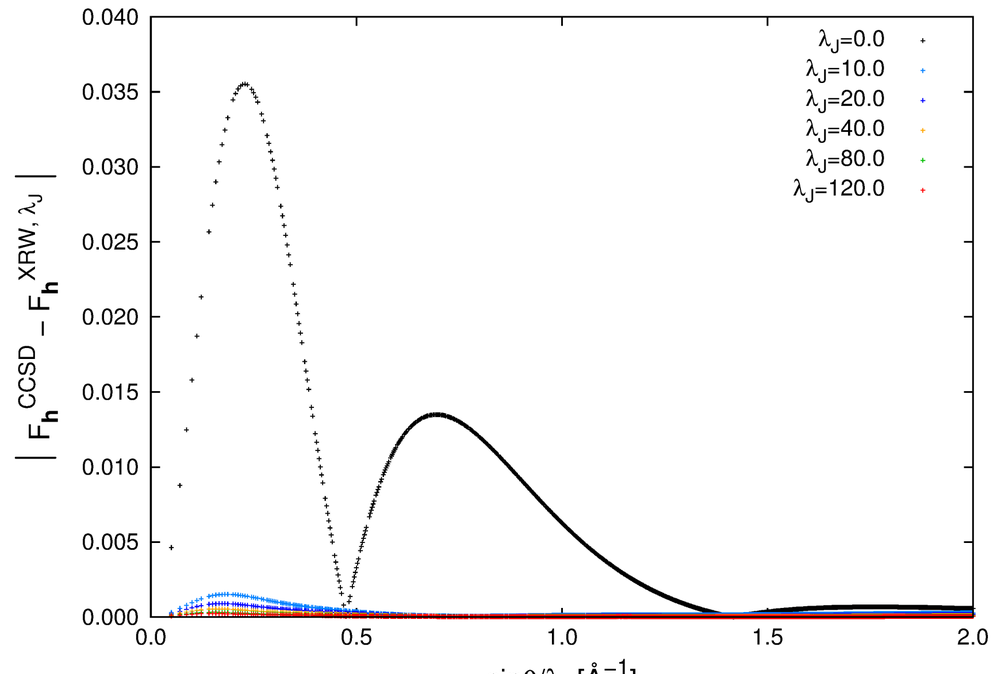

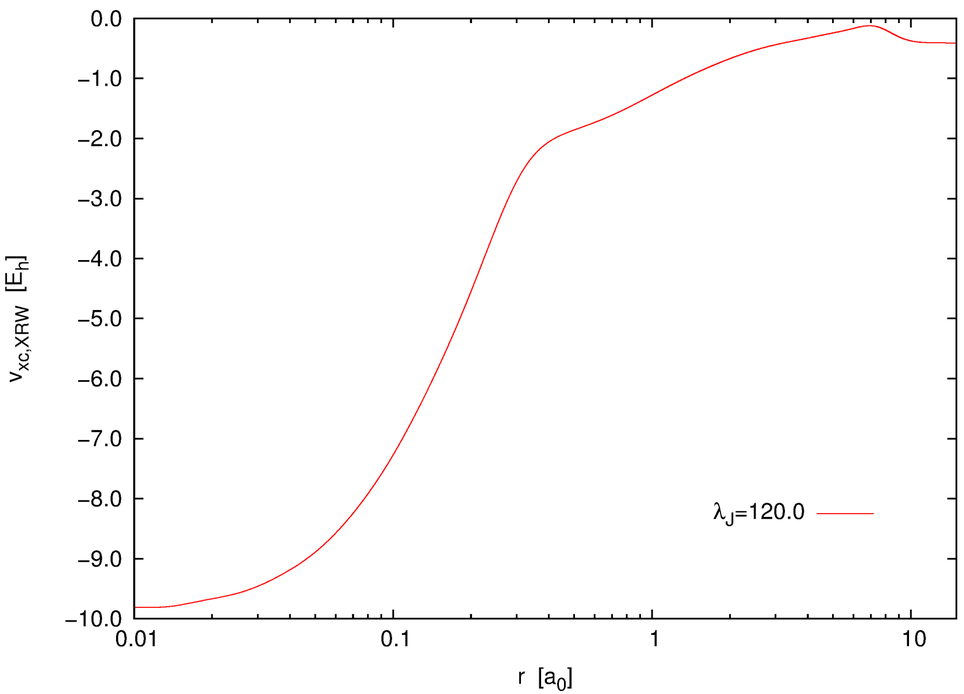

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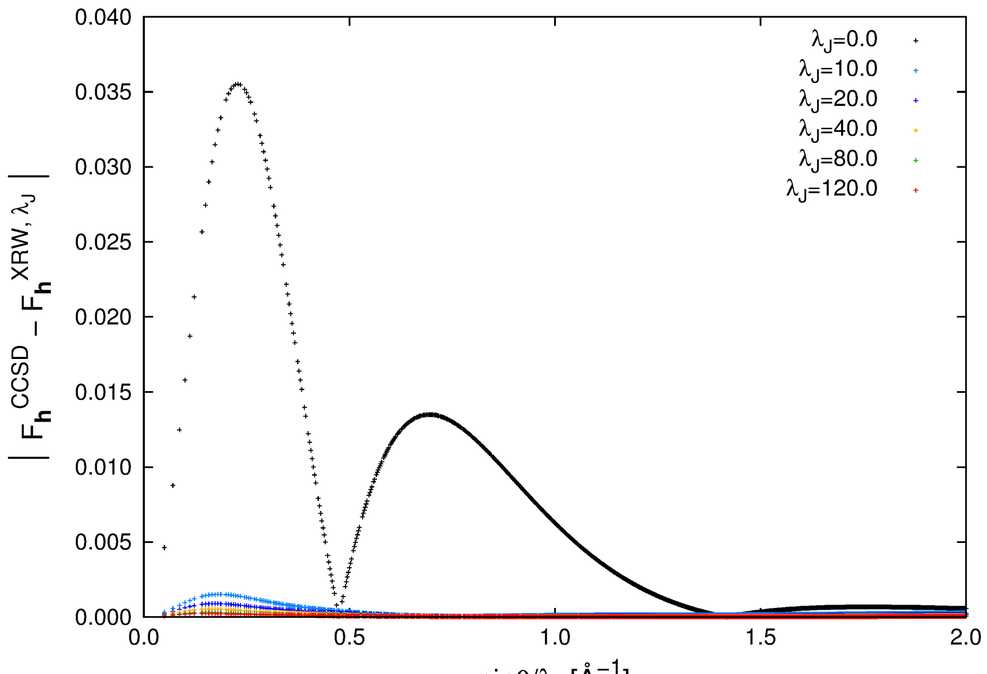

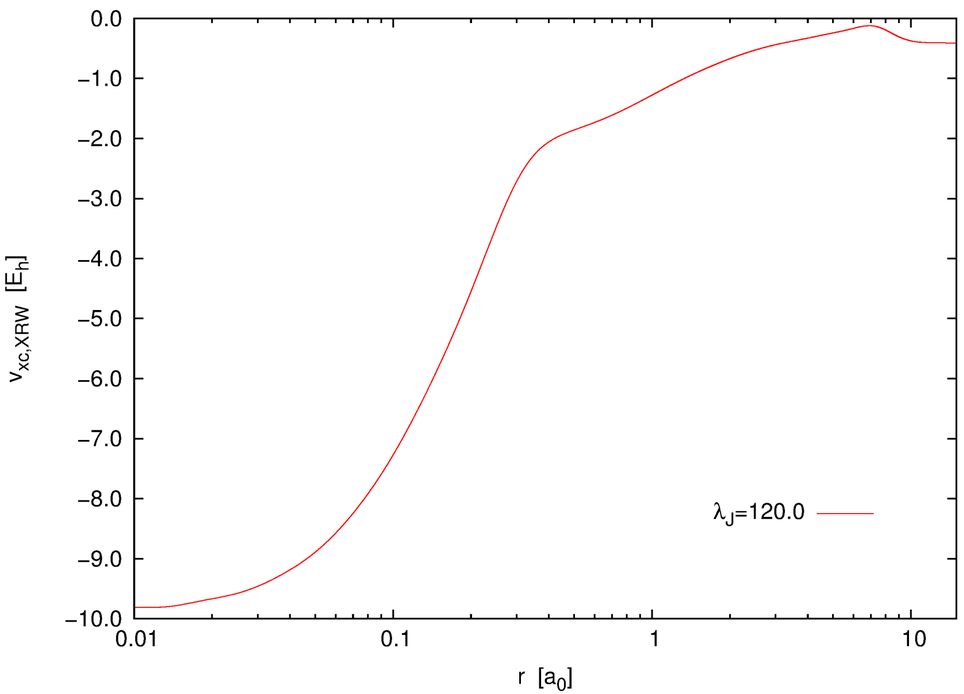

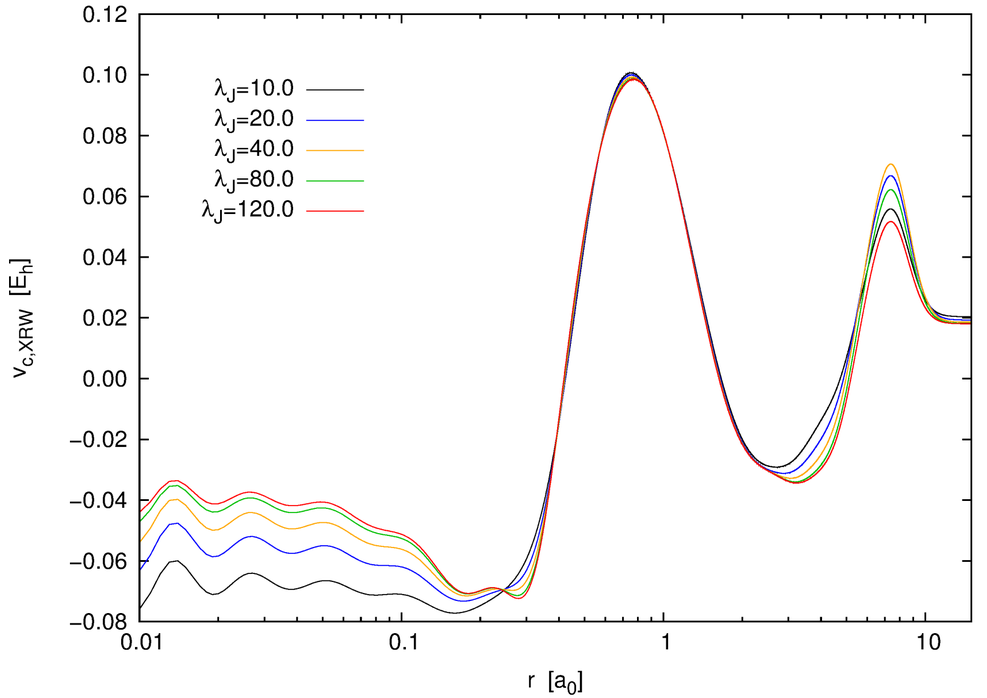

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Size of the fictitious cubic unit-cell: 7.5 $\mathrm{\AA}$

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λ_J	$\int \lvert\Delta\rho(\mathbf{r})\rvert \, d\mathbf{r}$ (e)
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2.5	0.0145
5.0	0.0126
10.0	0.0116
20.0	0.0111
26.7	0.0110

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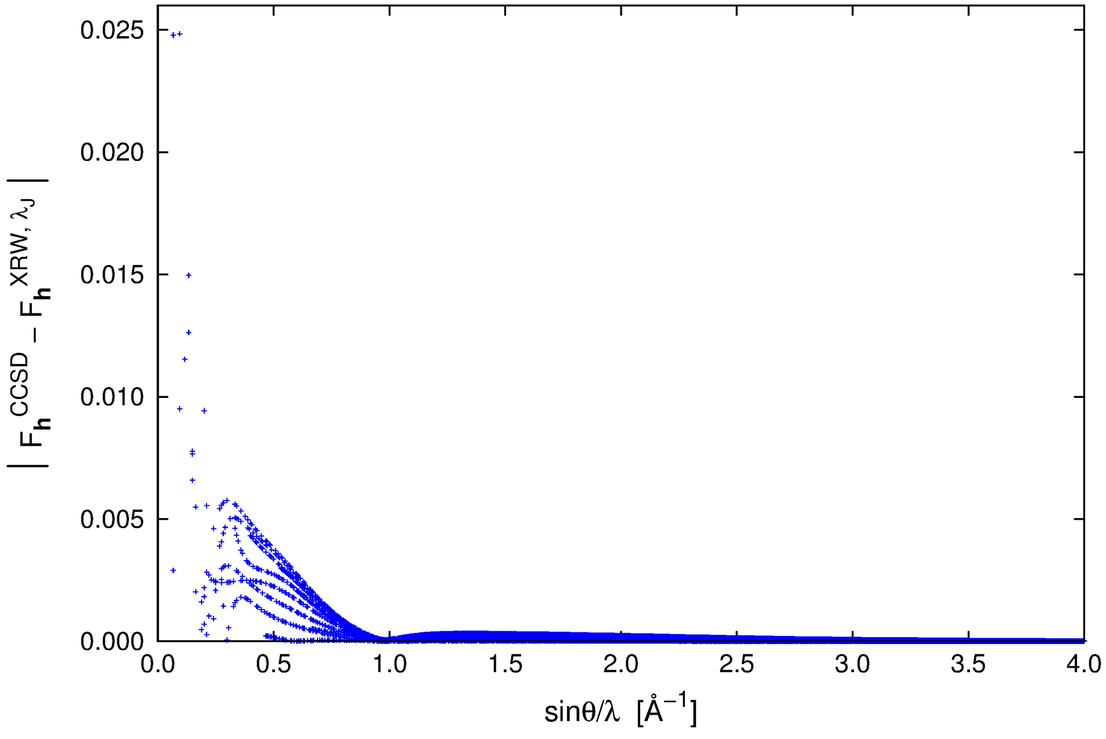
Differences between CCSD and XRW structure factor amplitudes (λ_J=0.0)



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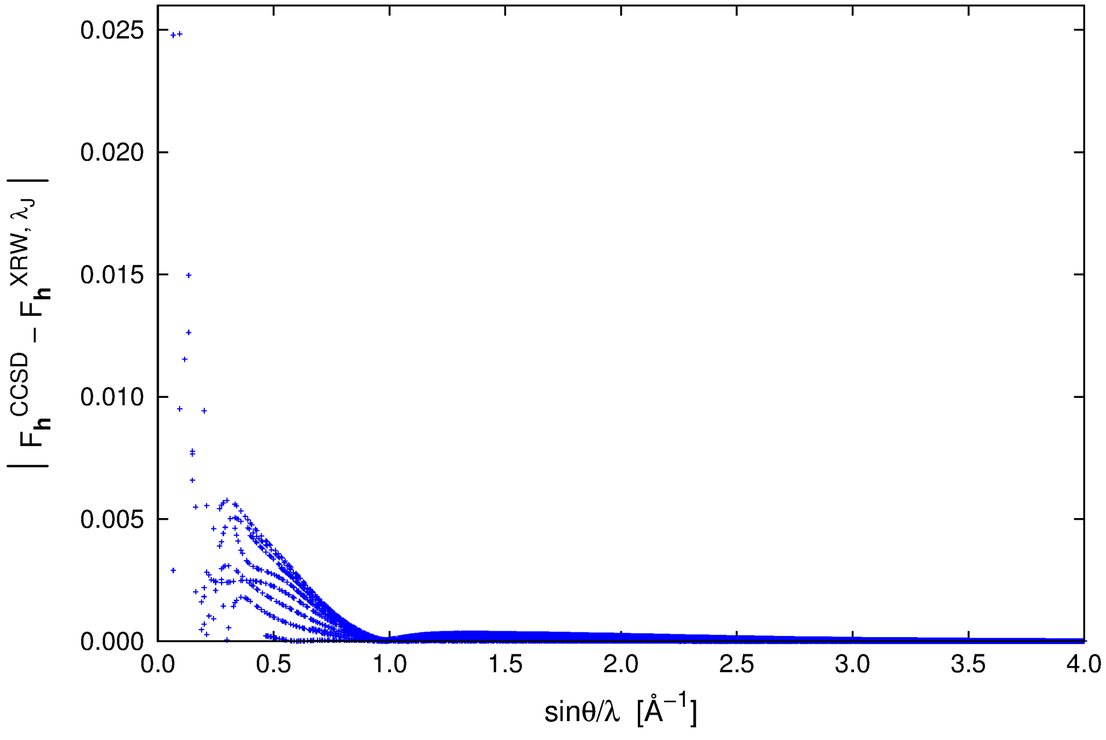
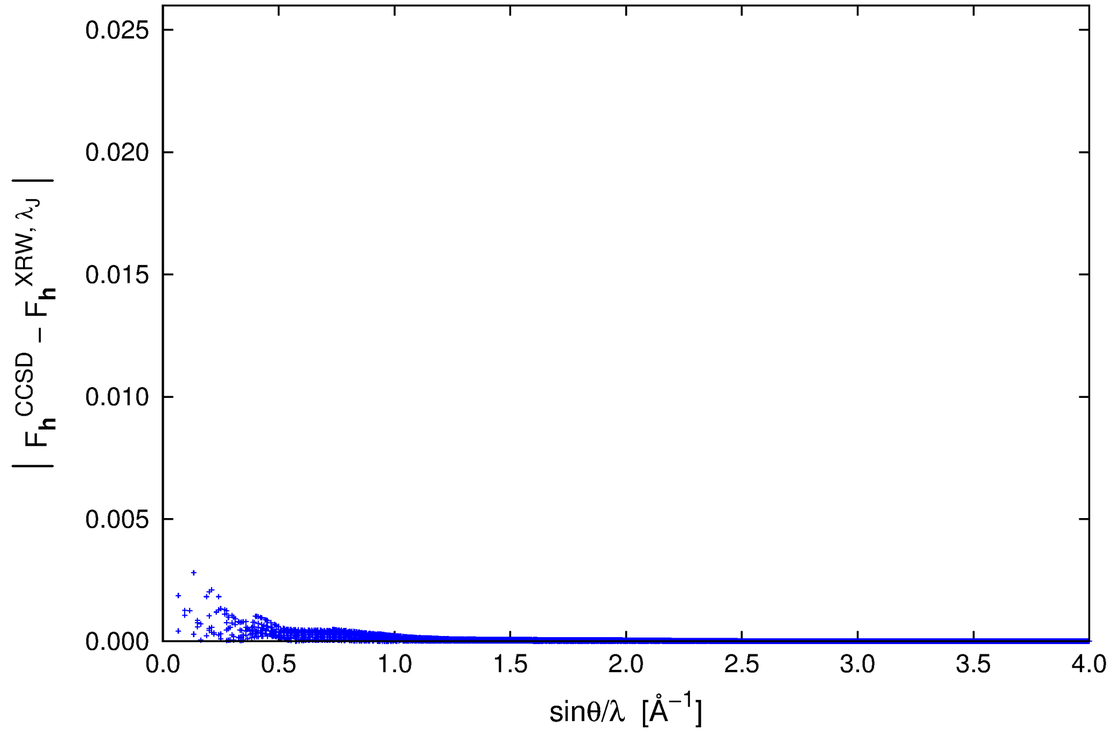


Differences between CCSD and XRW structure factor amplitudes (λ_J=26.7)



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Type of X-ray structure factors: gas-phase theoretically generated

Level of theory / basis set: CCSD / u6-311G*

Size of the fictitious cubic unit-cell: 7.5 Å

Limit of structure factor resolution: 4.0 $Å^{-1}$ (namely, 0.125 Å)

λ_J	$\int \lvert\Delta\rho(\mathbf{r})\rvert \, d\mathbf{r}$ (e)
0.0	0.0700
2.5	0.0145
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10.0	0.0116
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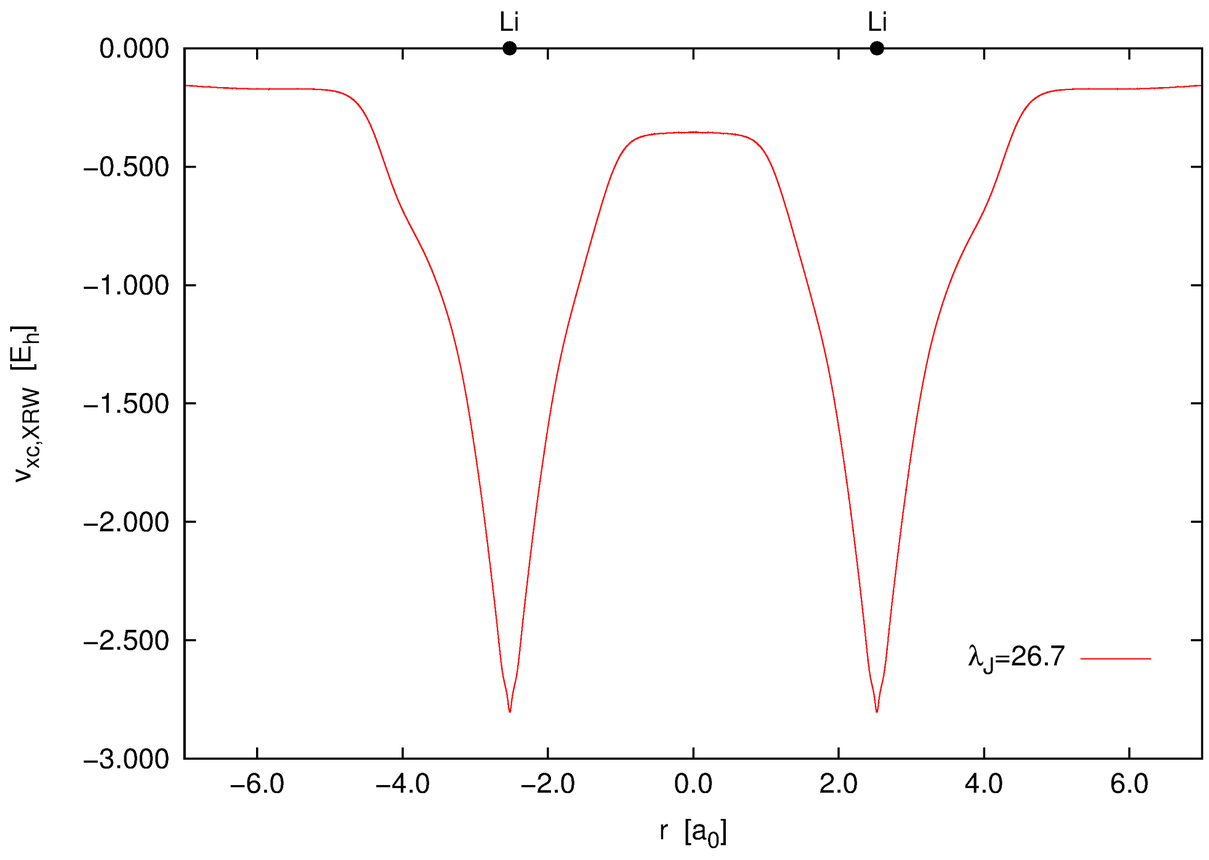

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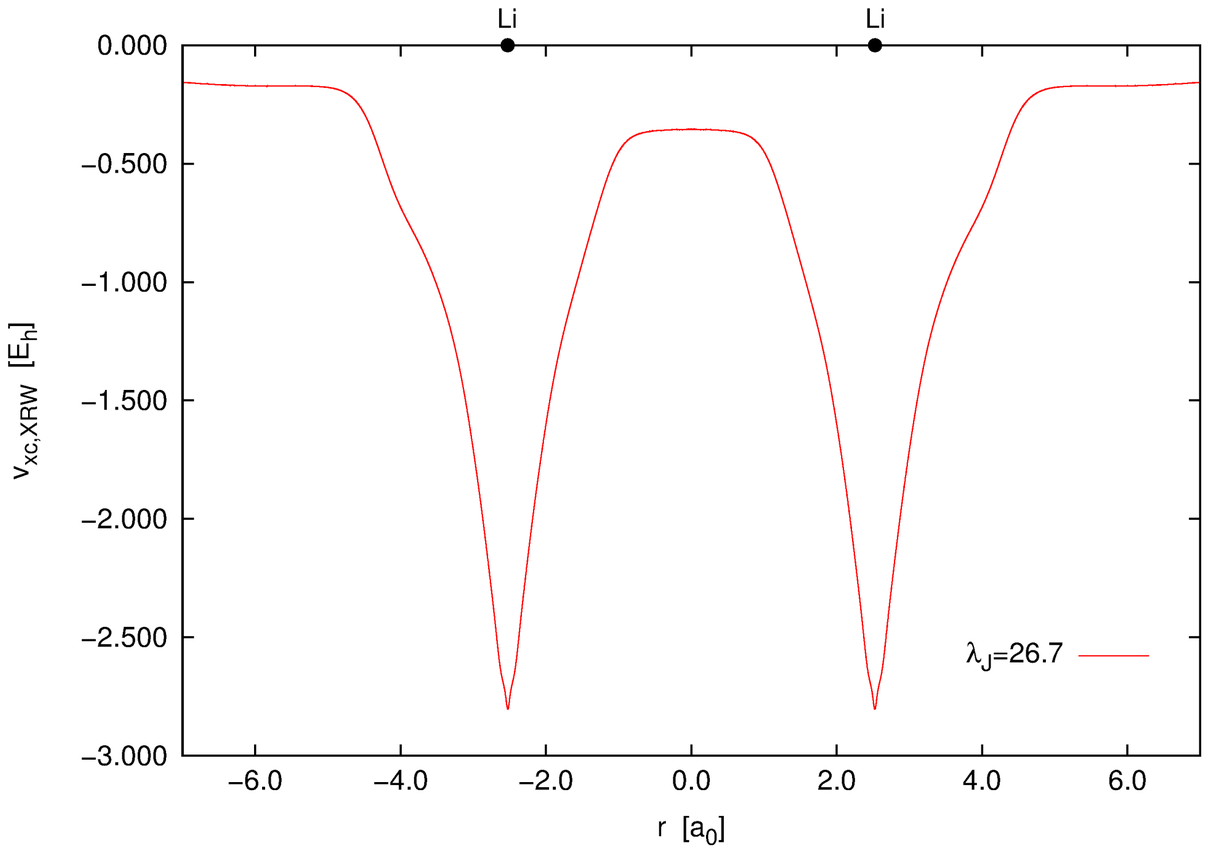

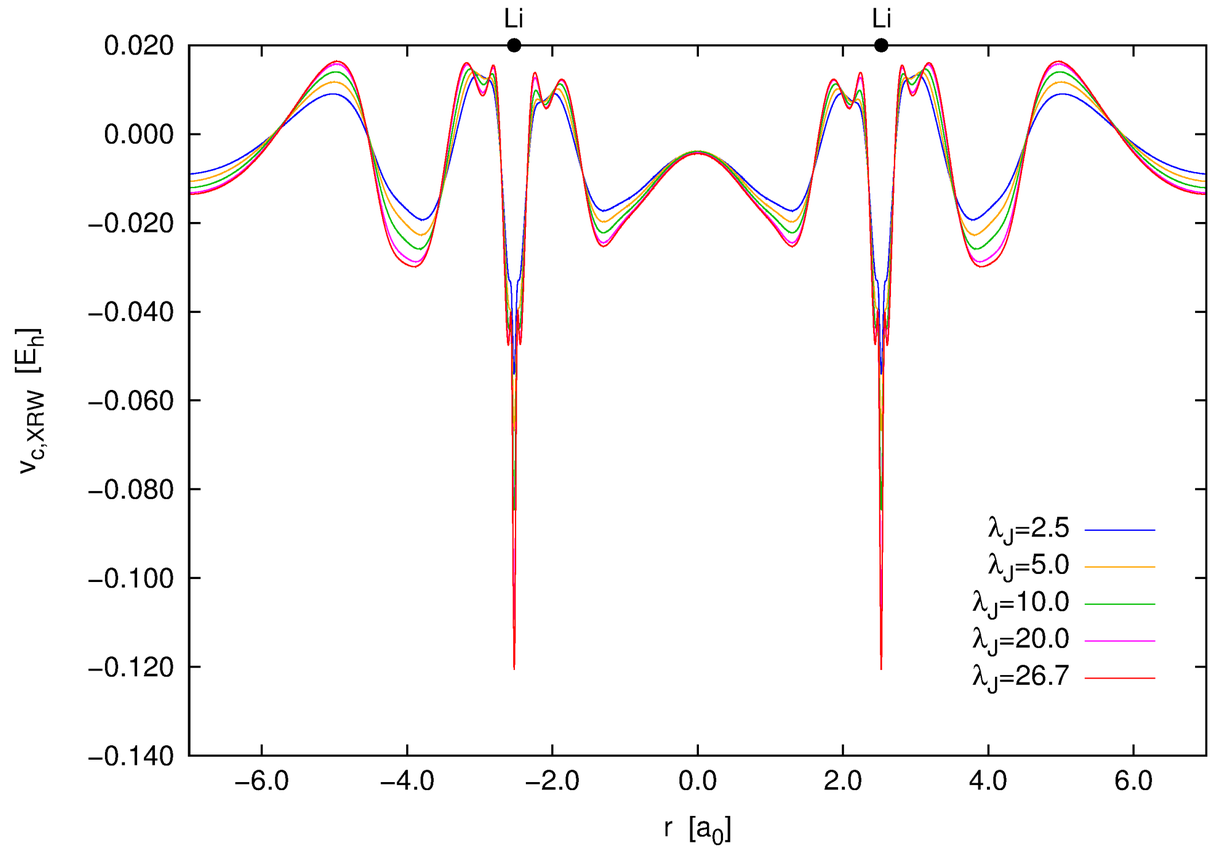

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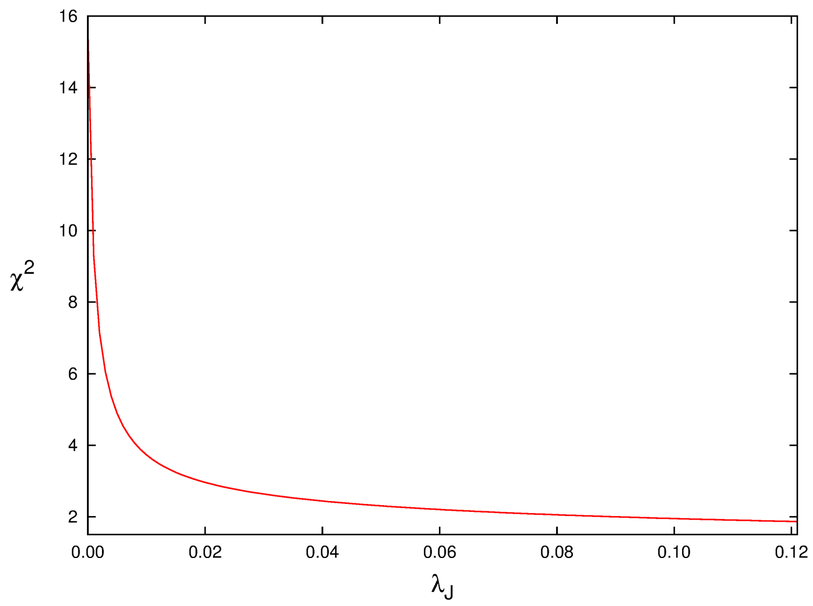

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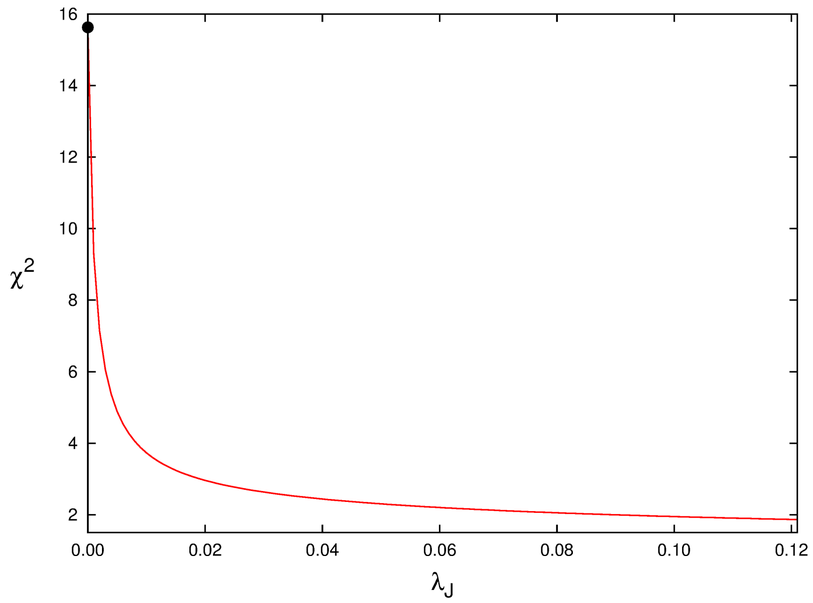

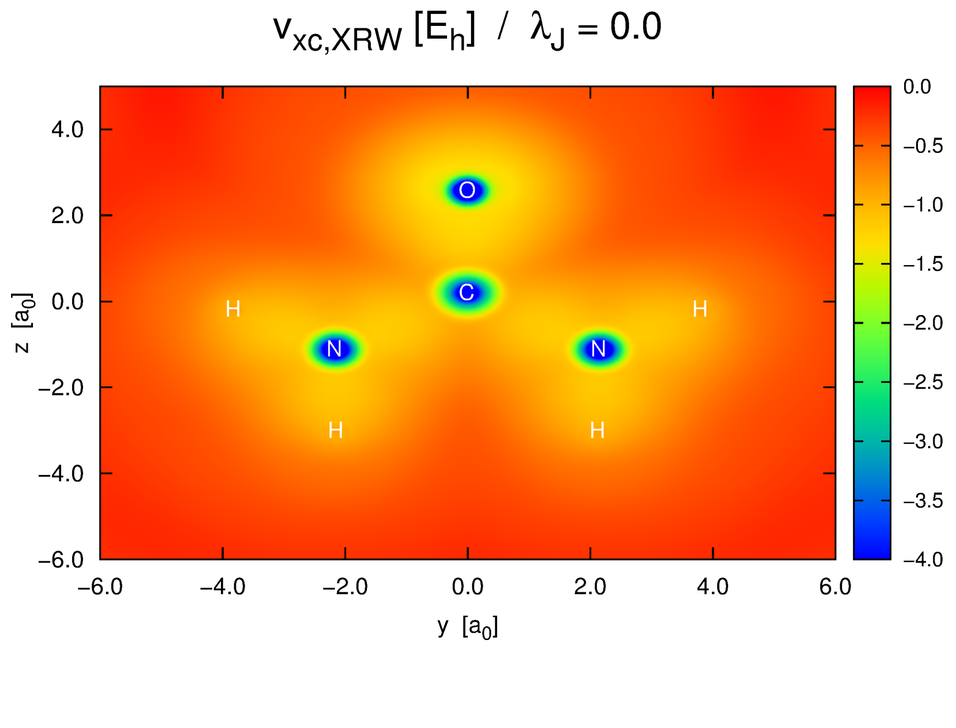

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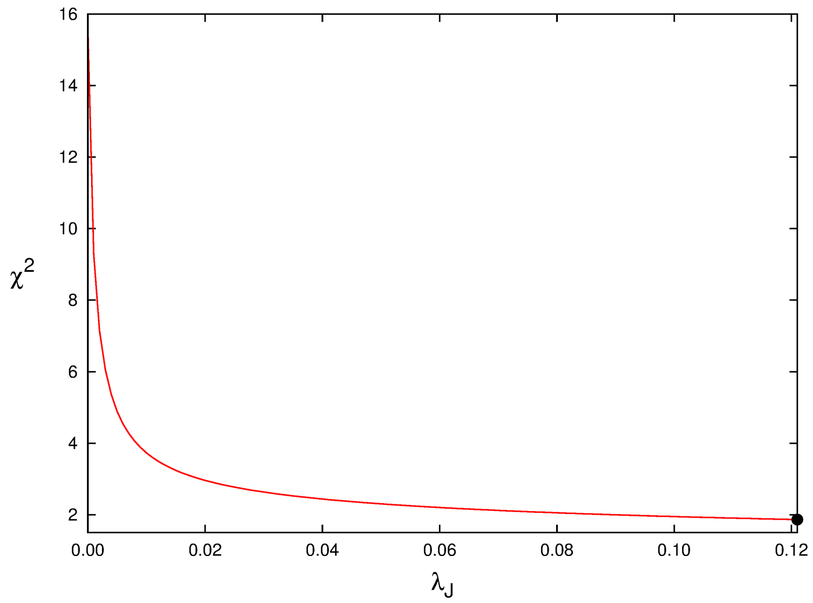

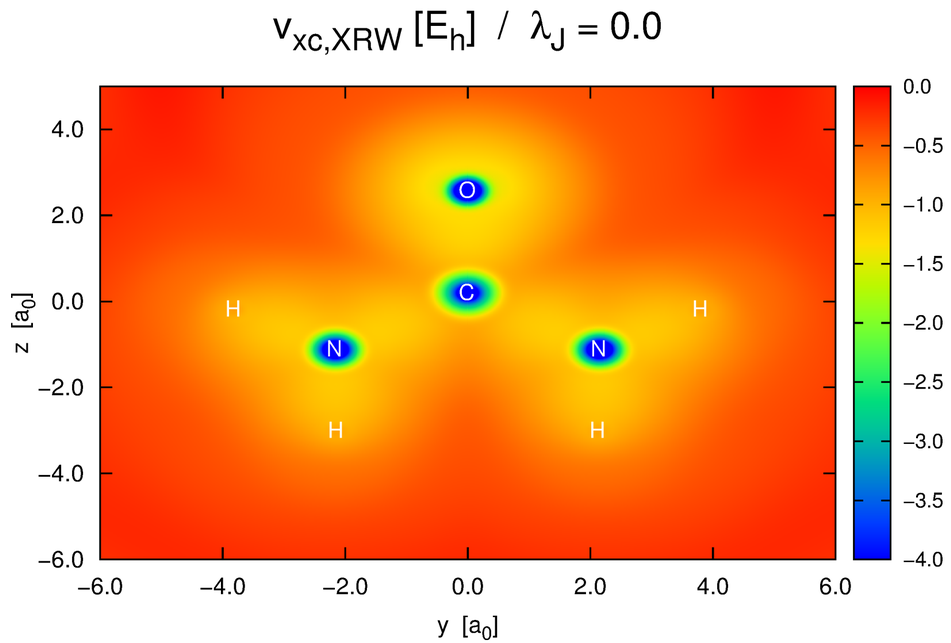

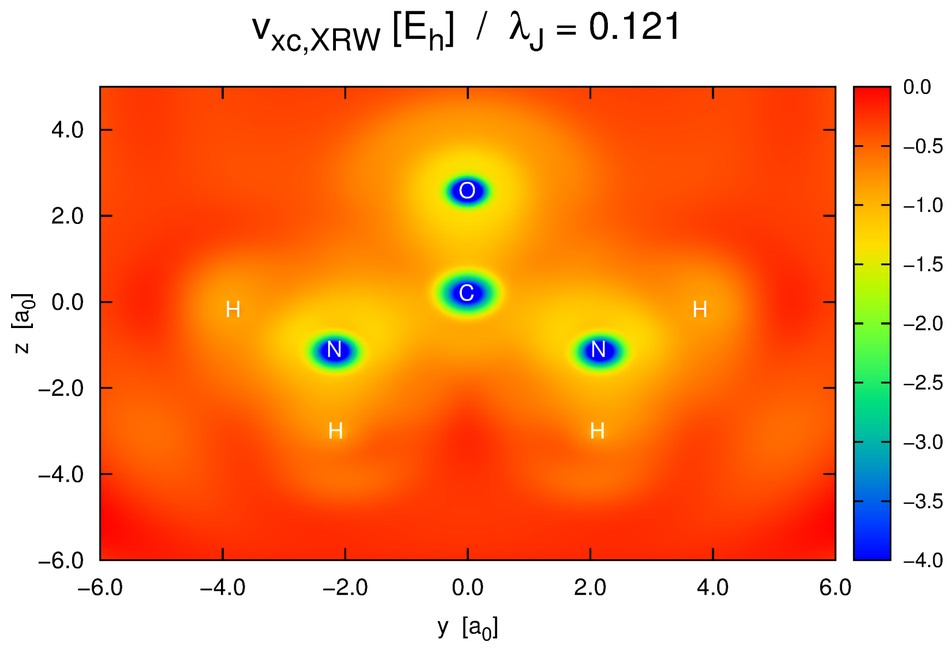

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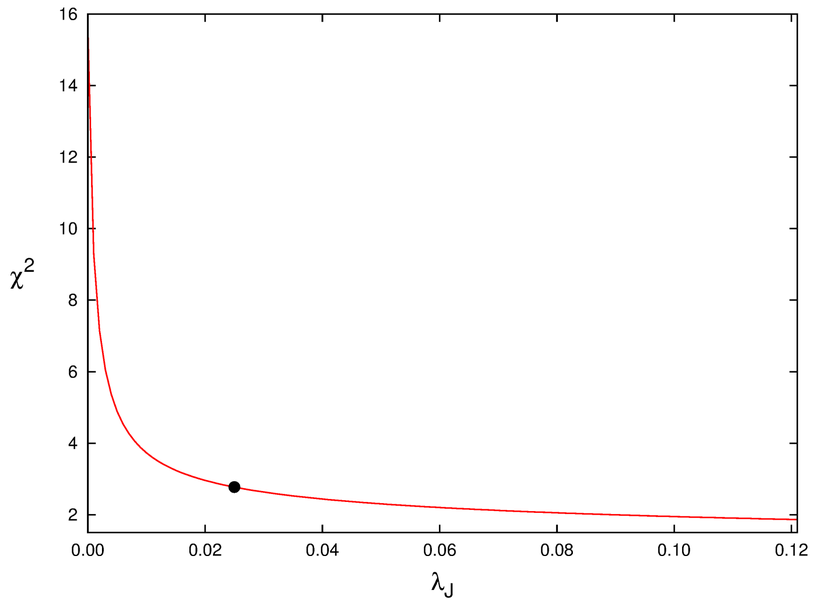

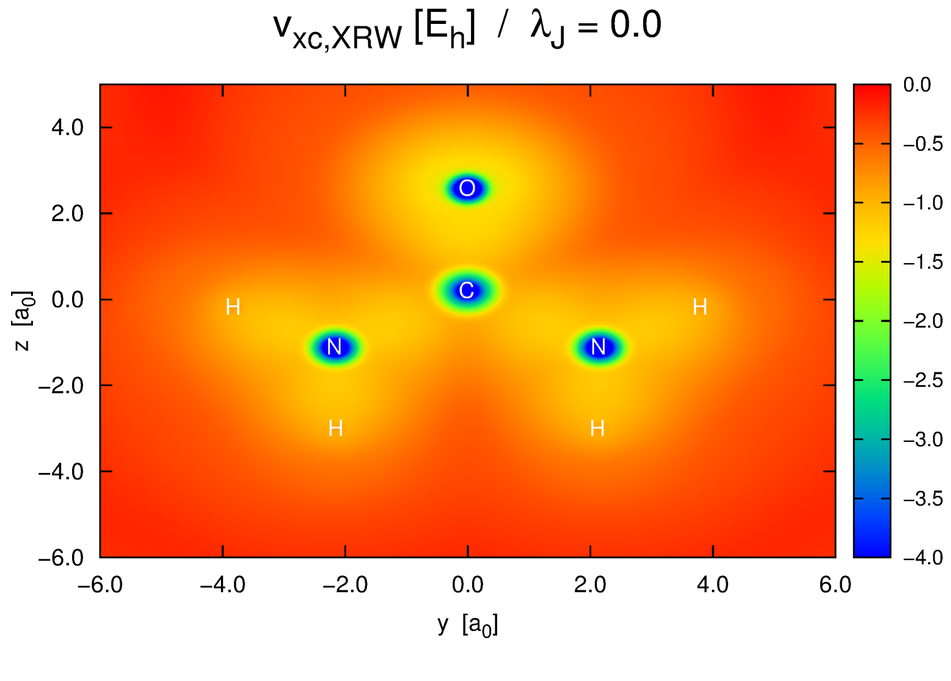

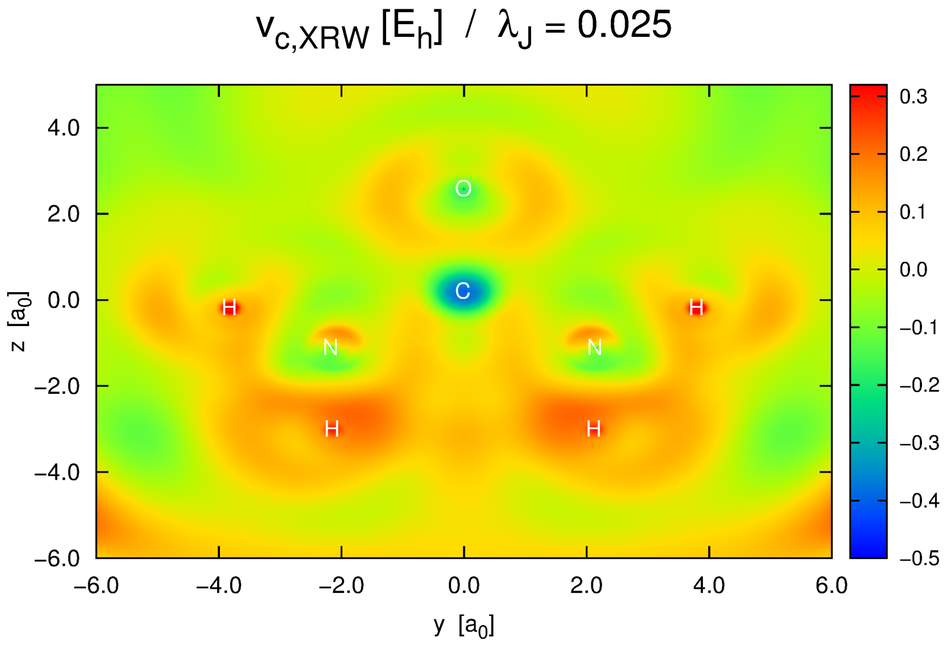

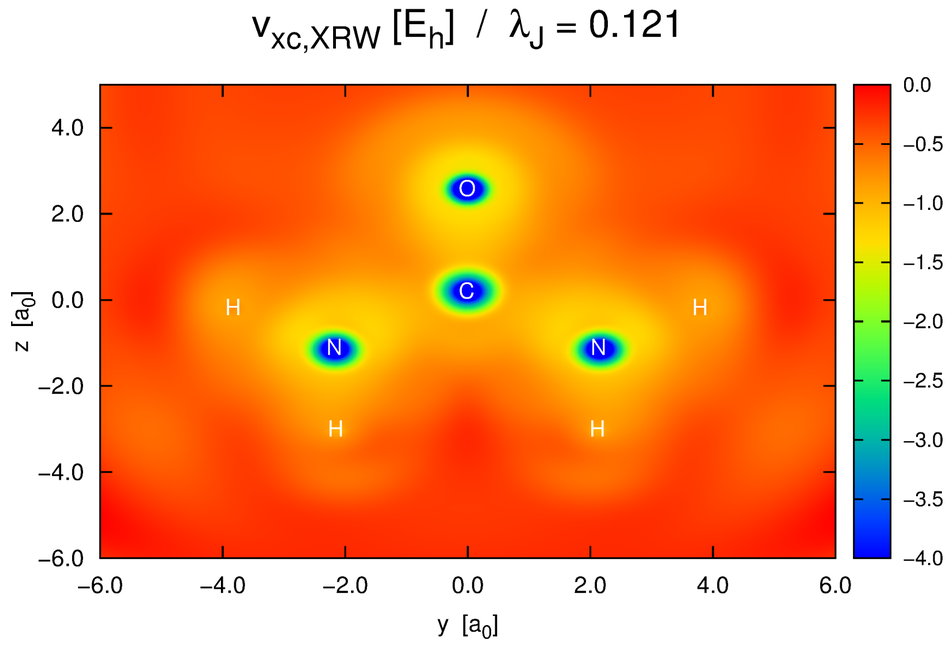

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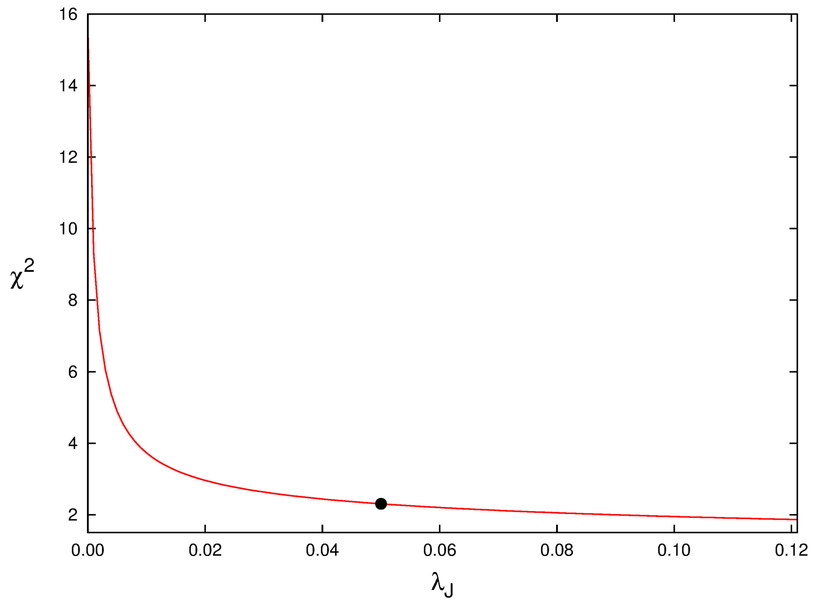

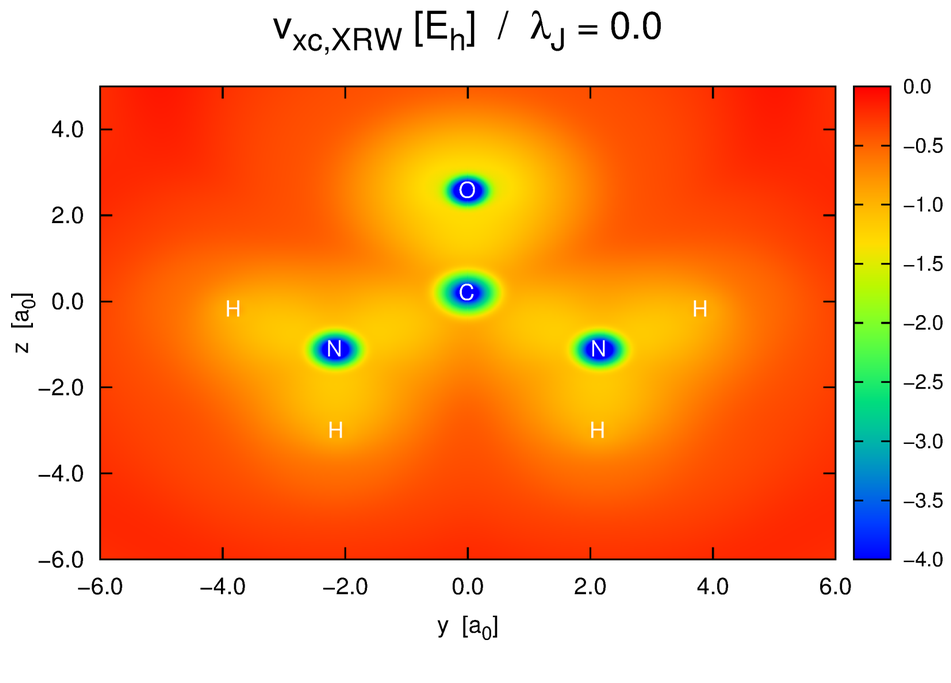

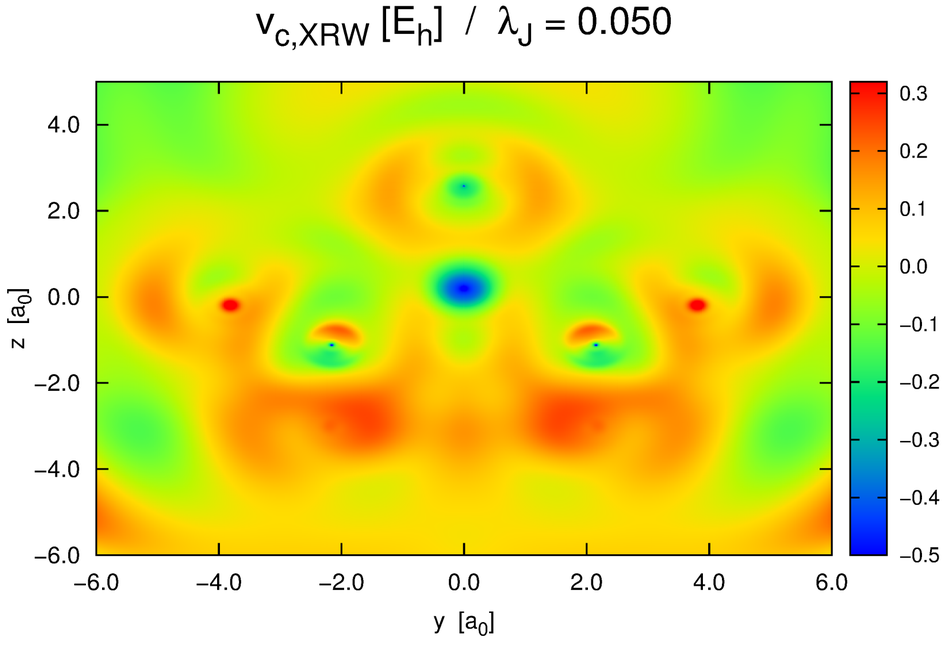

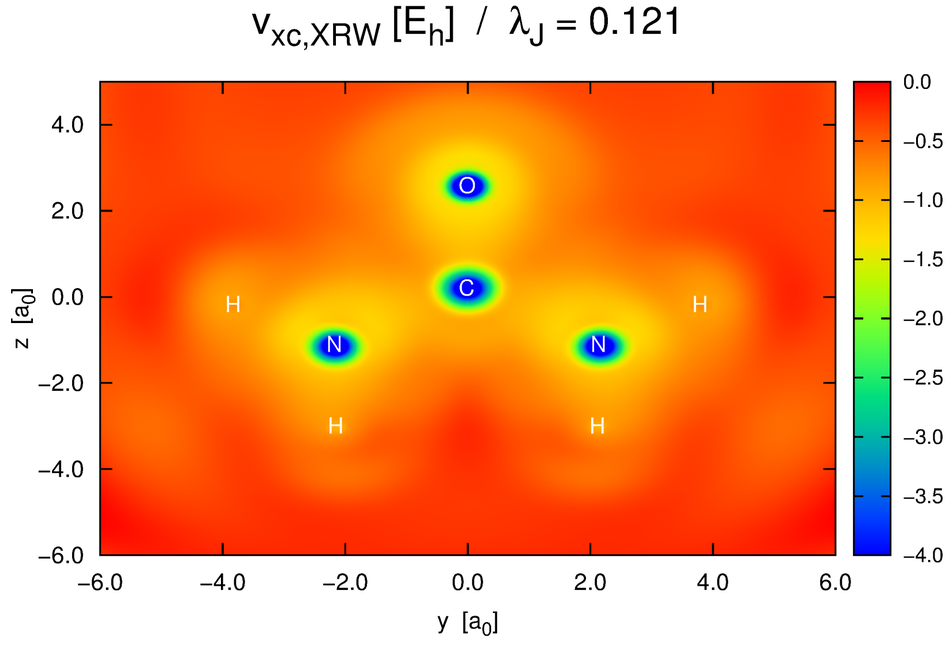

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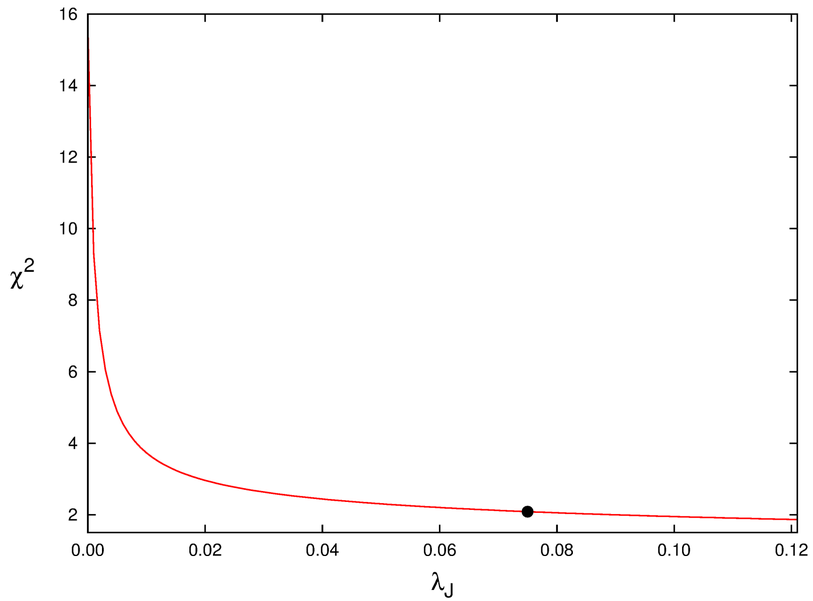

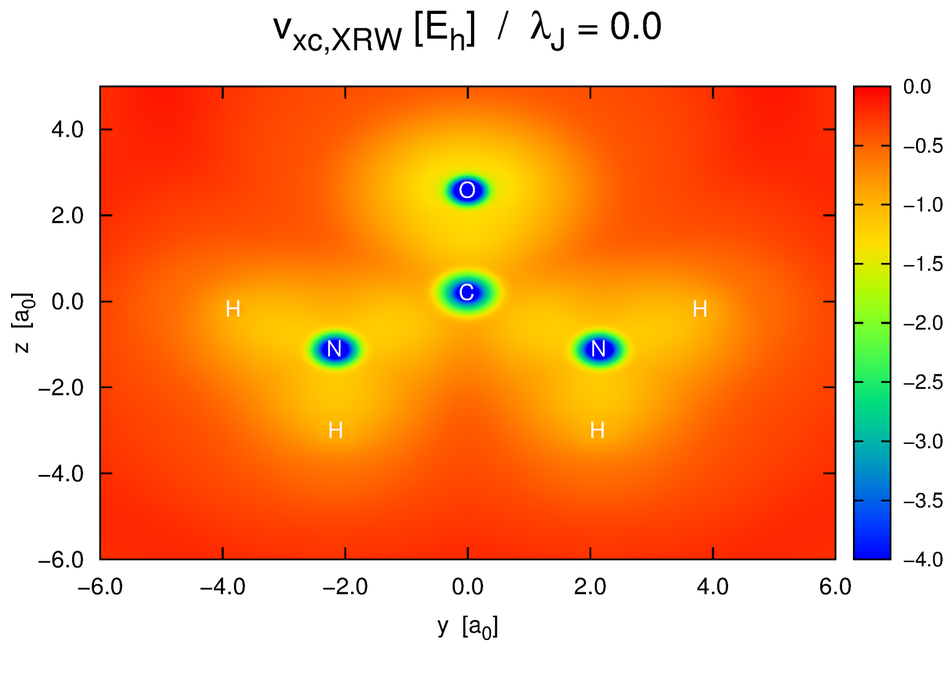

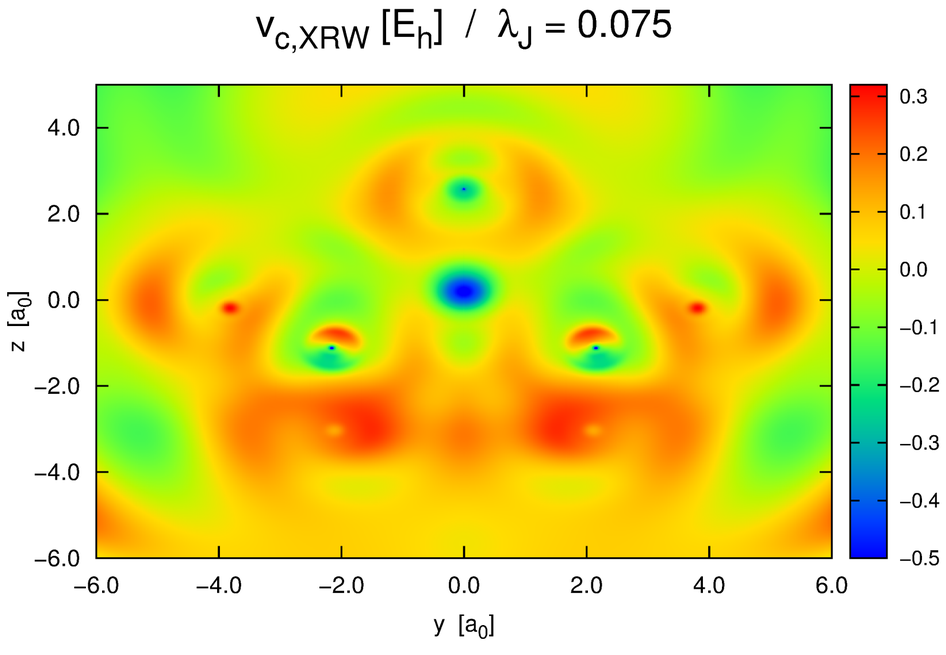

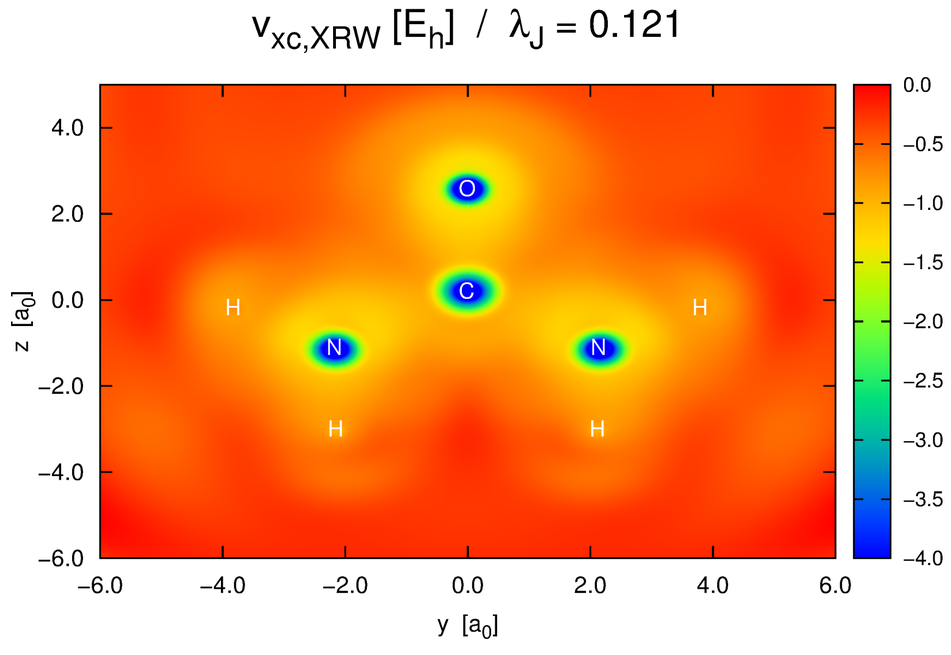

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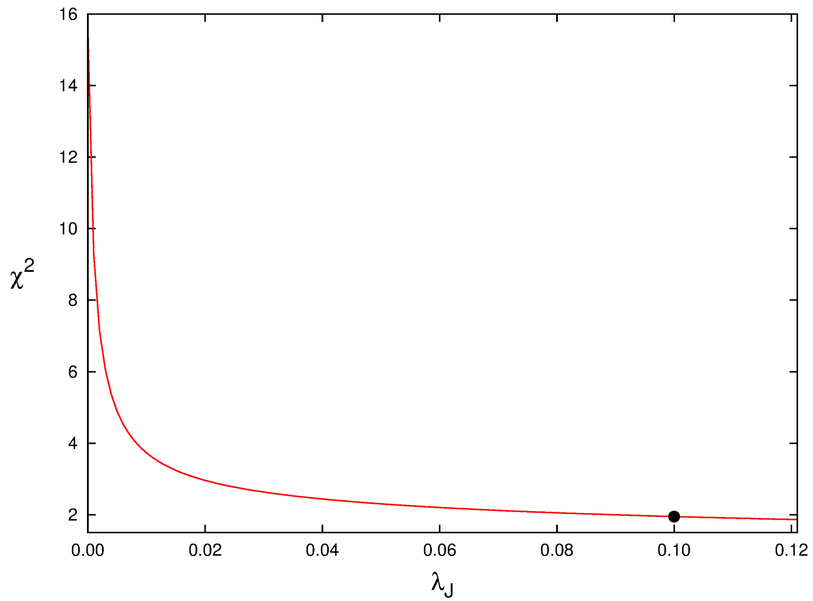

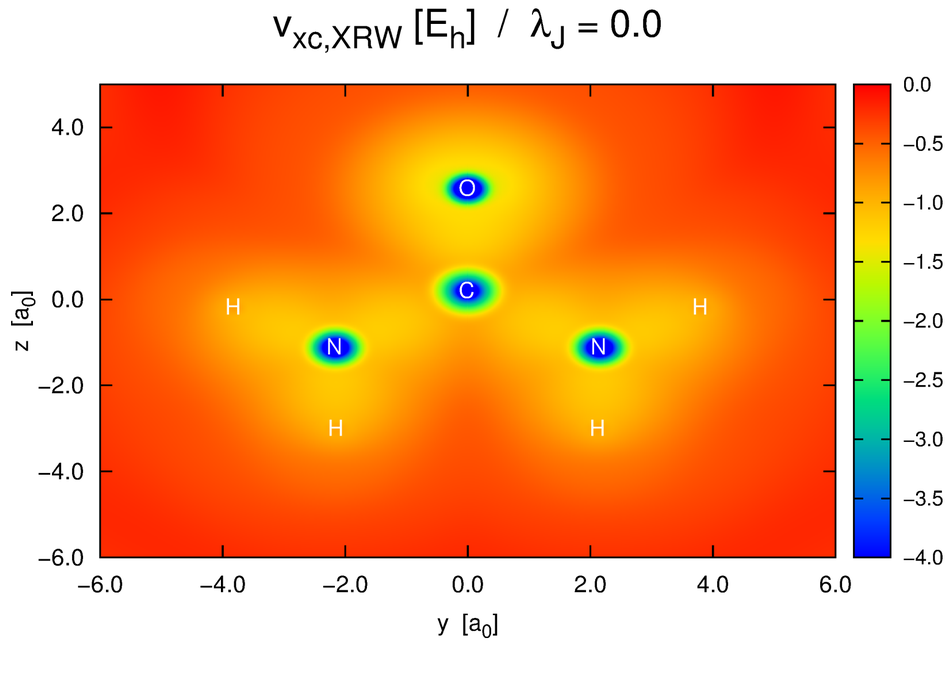

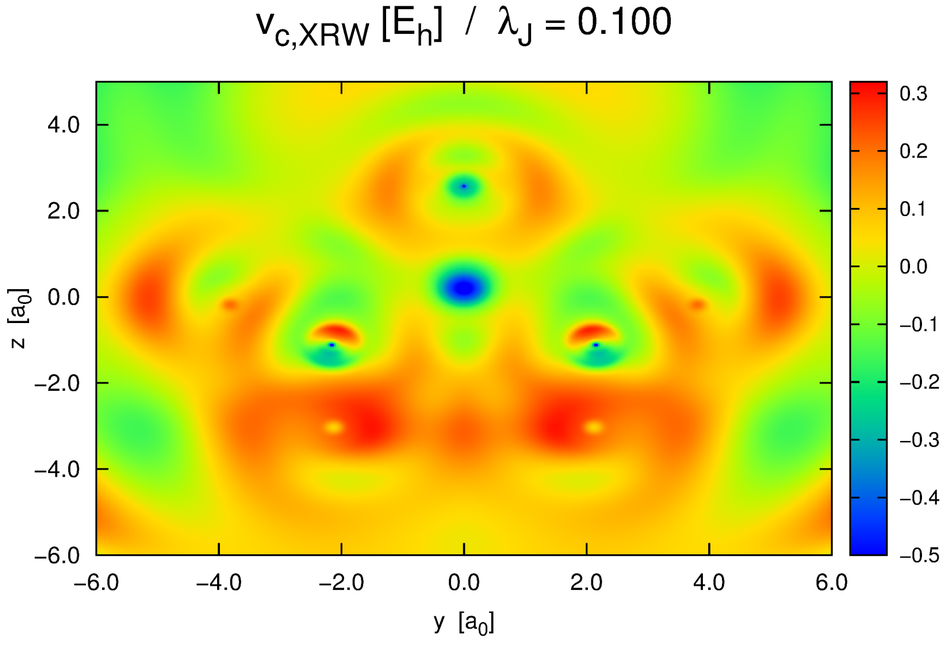

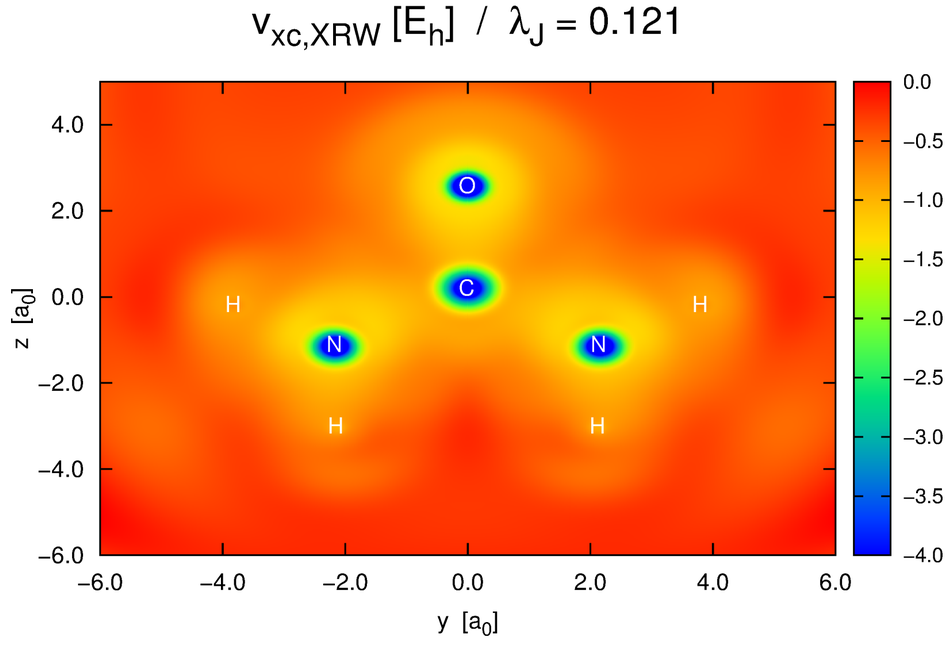

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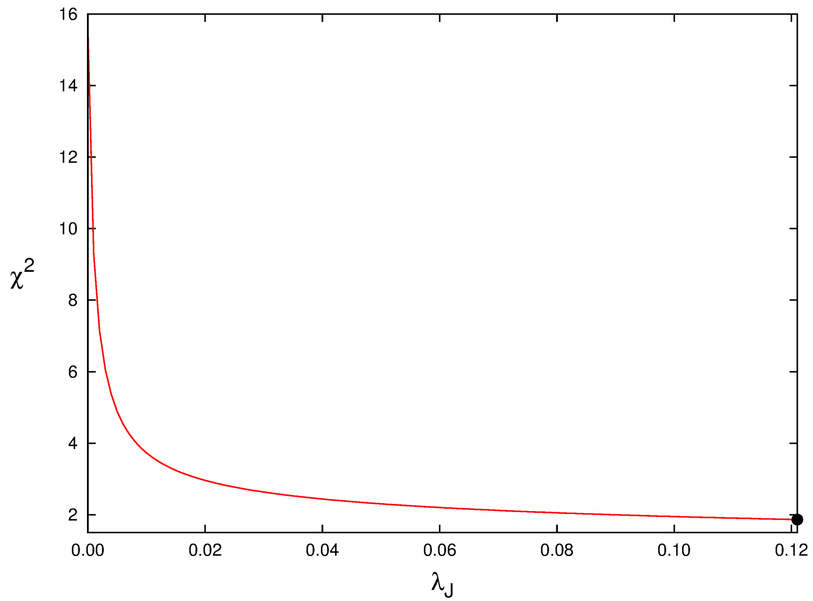

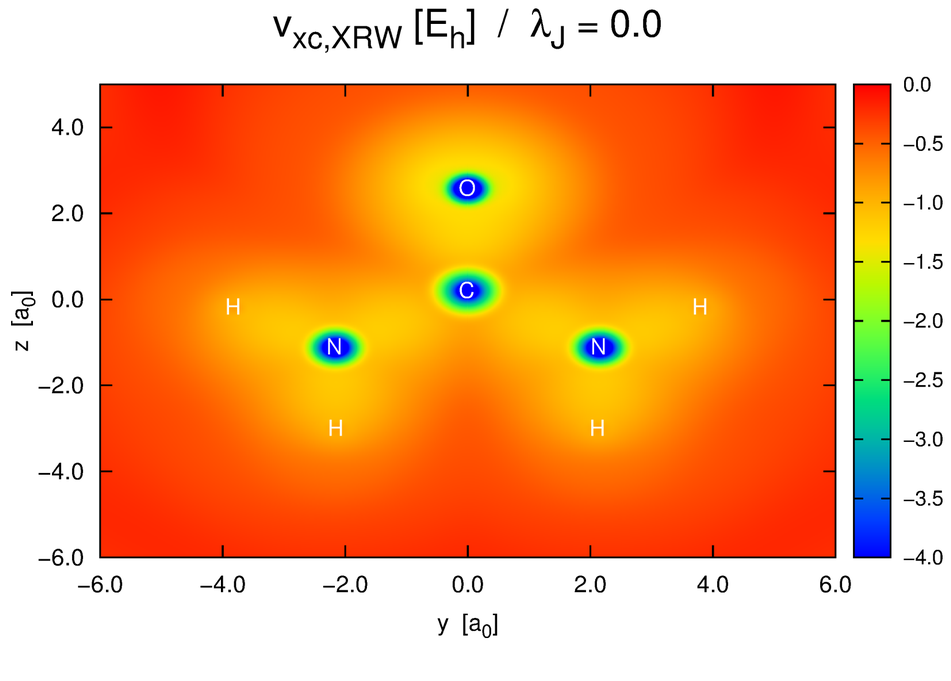

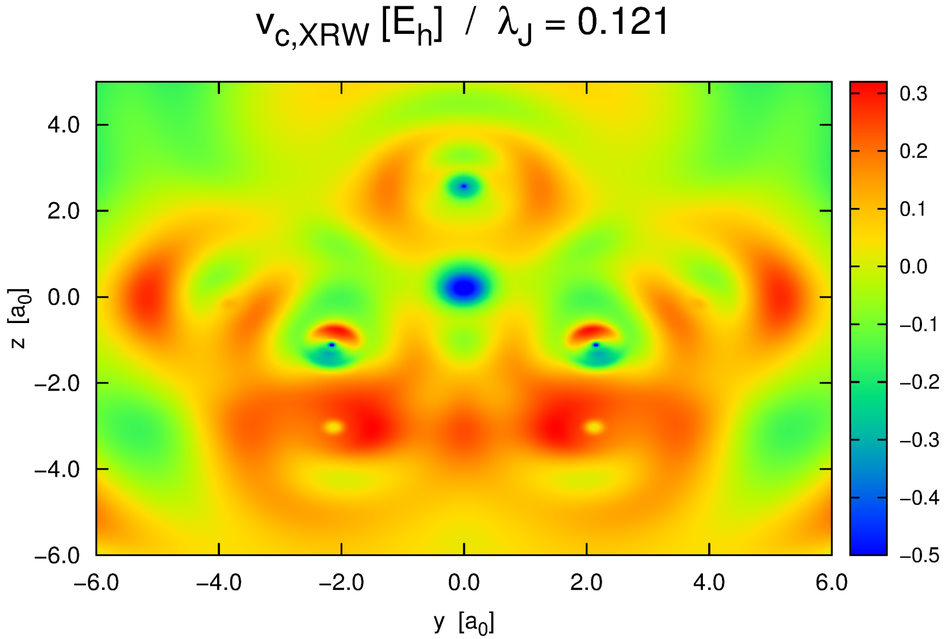

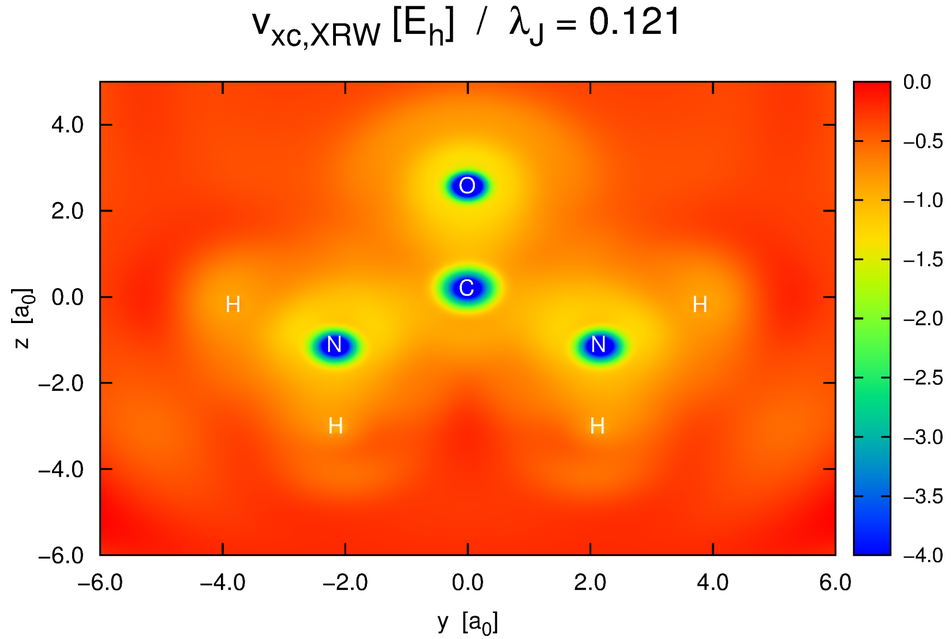

xc-Potentials from X-ray Data: First Conclusions and Outlooks

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Methods with a strong interplay between quantum chemistry and X-ray diffraction measurements

X-ray diffraction data are directly integrated into quantum mechanical calculations to enhance the information content of the wavefunction

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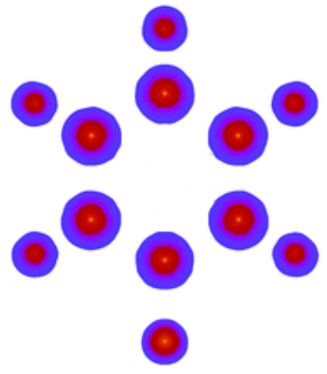

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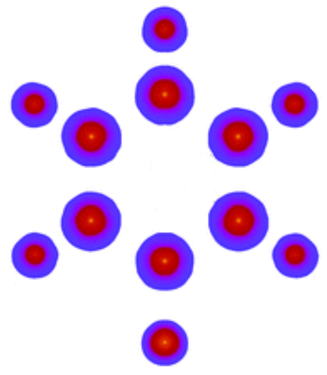

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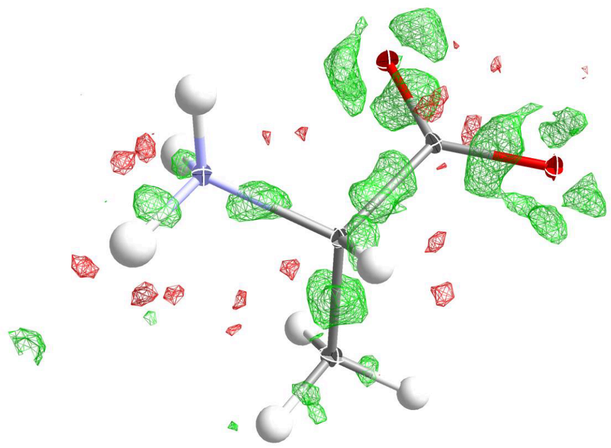

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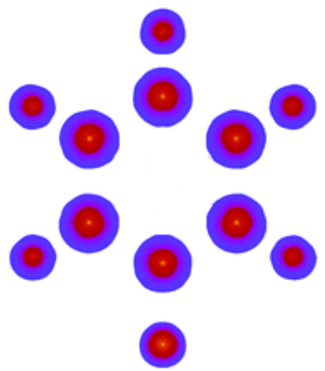

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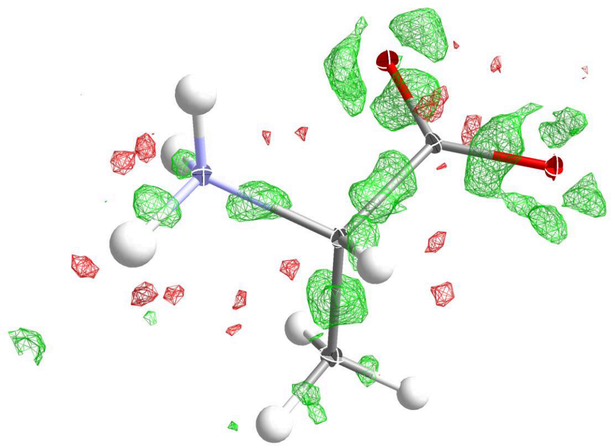

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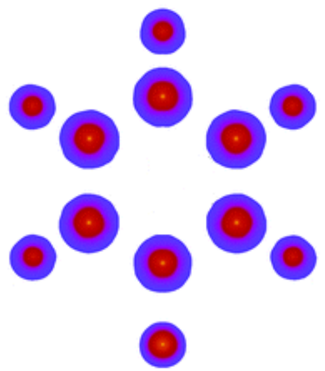

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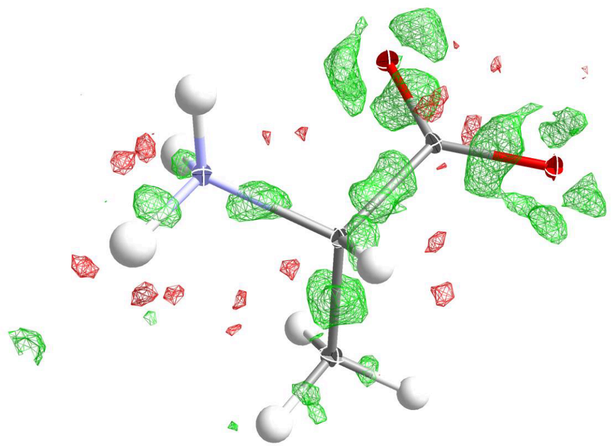

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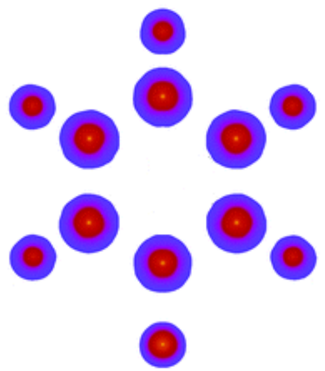

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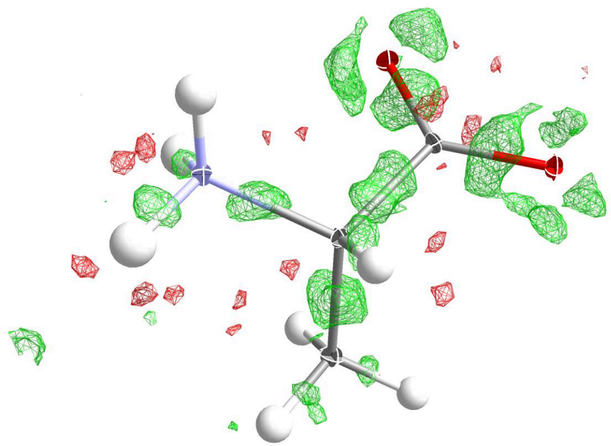
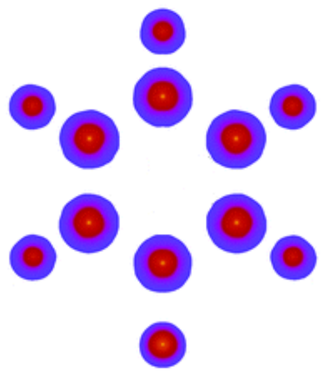


Residual density of L-Alanine after IAM refinement
(from -0.16 eÅ^{-3} to +0.16 eÅ^{-3})



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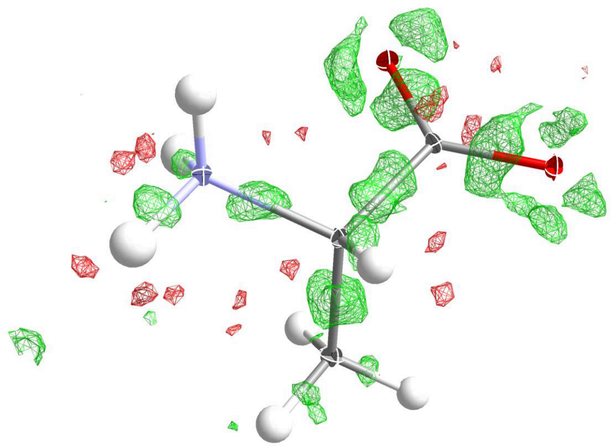

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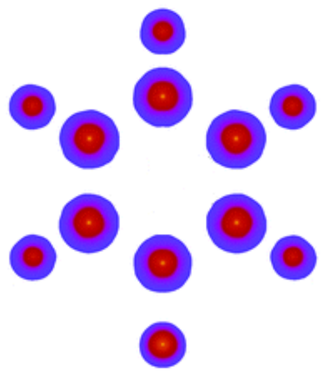

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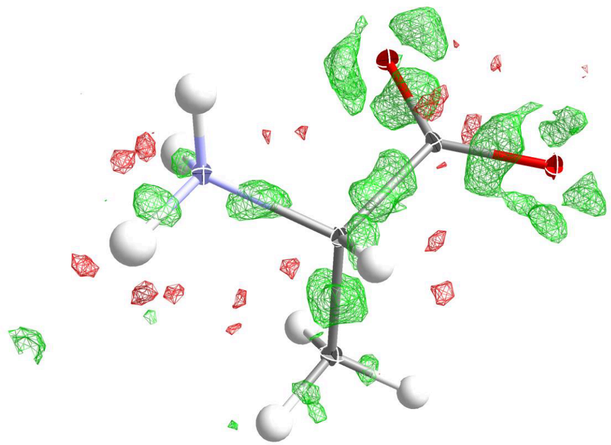

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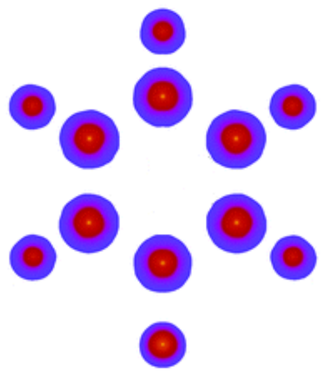

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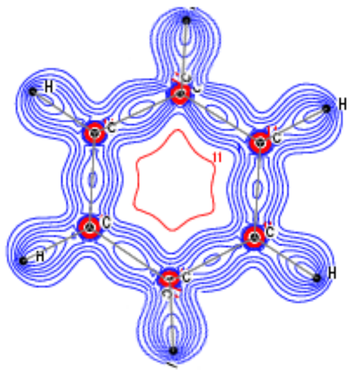
⟶ **Aspherical atom models**, where the deformations due to chemical bonding are implicitly considered



- Chemical bonds and lone pairs are taken into account
- Improvement of E-H bond lengths compared to the IAM values

An Emerging Refinement Technique: the Hirshfeld Atom Refinement

Among the refinement techniques based on aspherical models, an emerging method is the **Hirshfeld Atom Refinement (HAR)**

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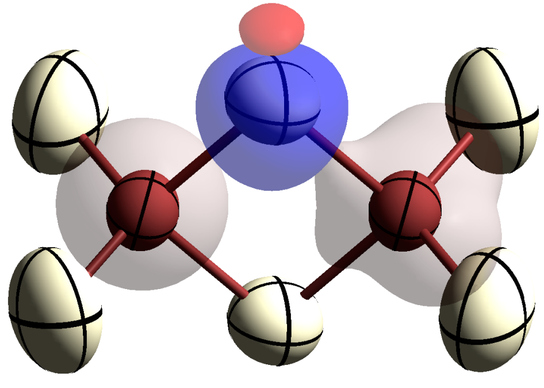

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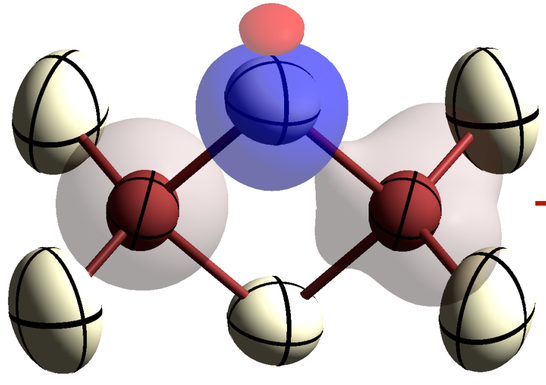

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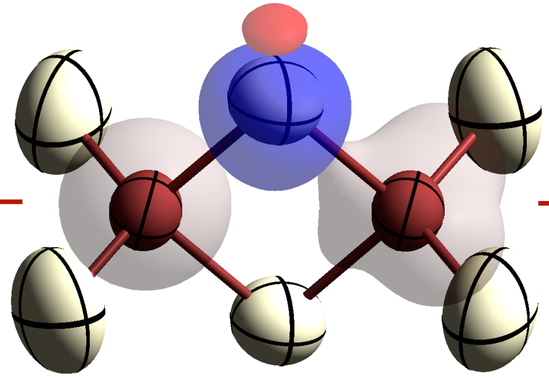

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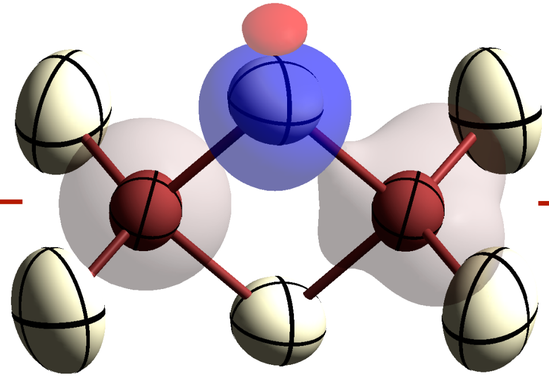

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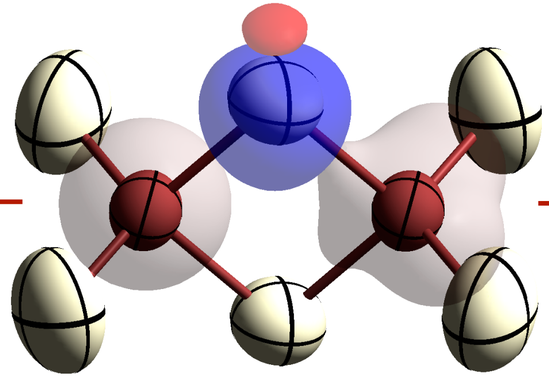

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Although quite small, the aspherical deformations are probably the reasons why HAR is so successful in determining the positions of hydrogen atoms from X-ray data

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Starting Atomic Positions (XYZ)

Quantum mechanical calculation

Partitioning of the electron density into Hirshfeld atoms and computation of the structure factors

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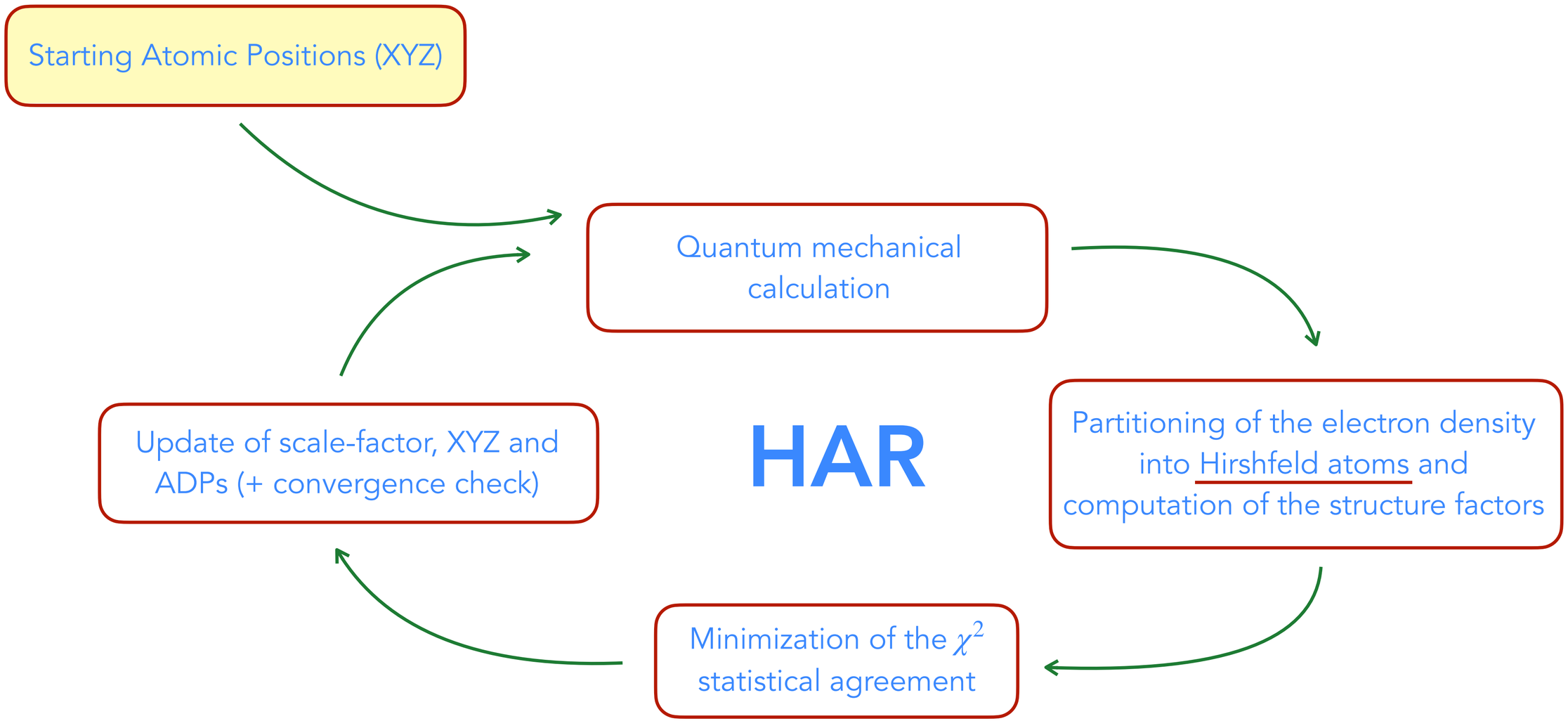

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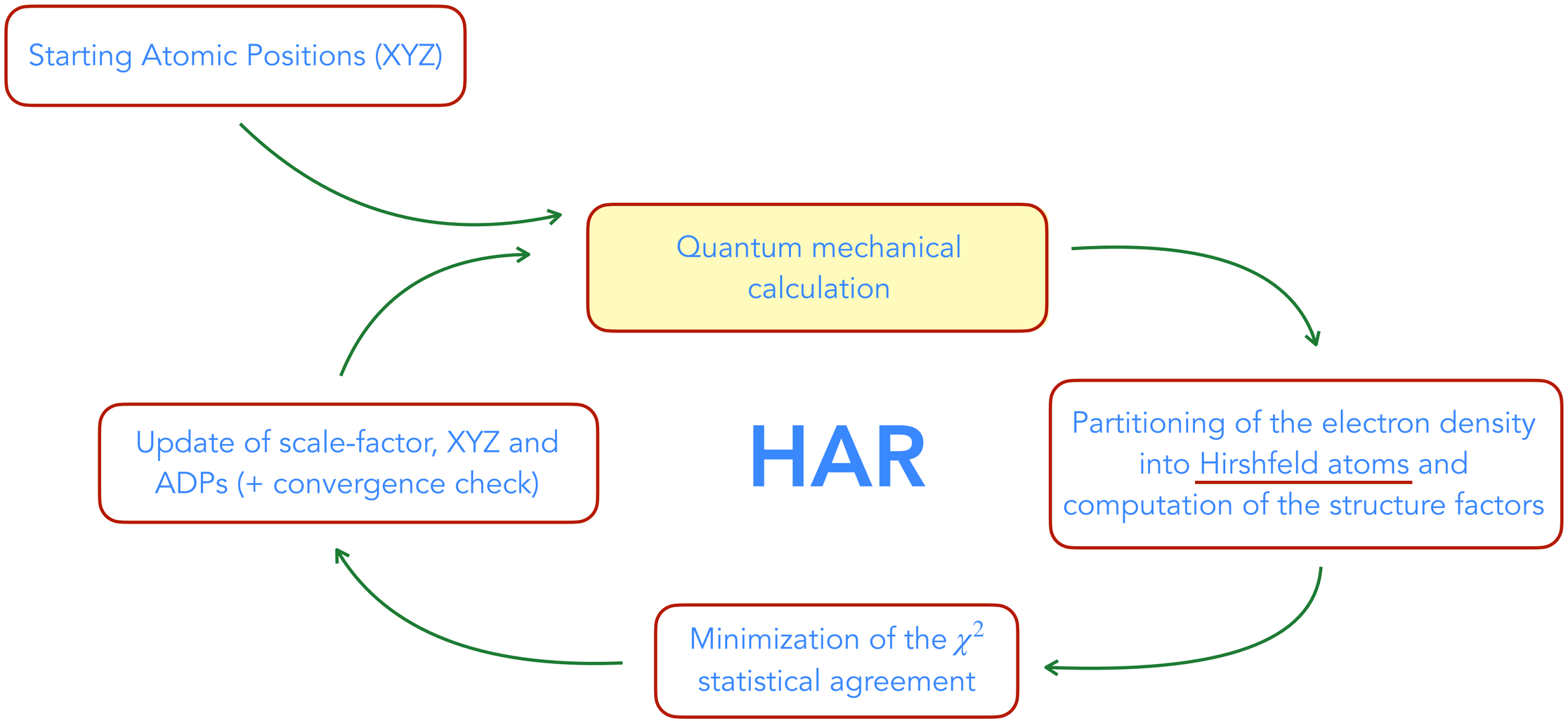

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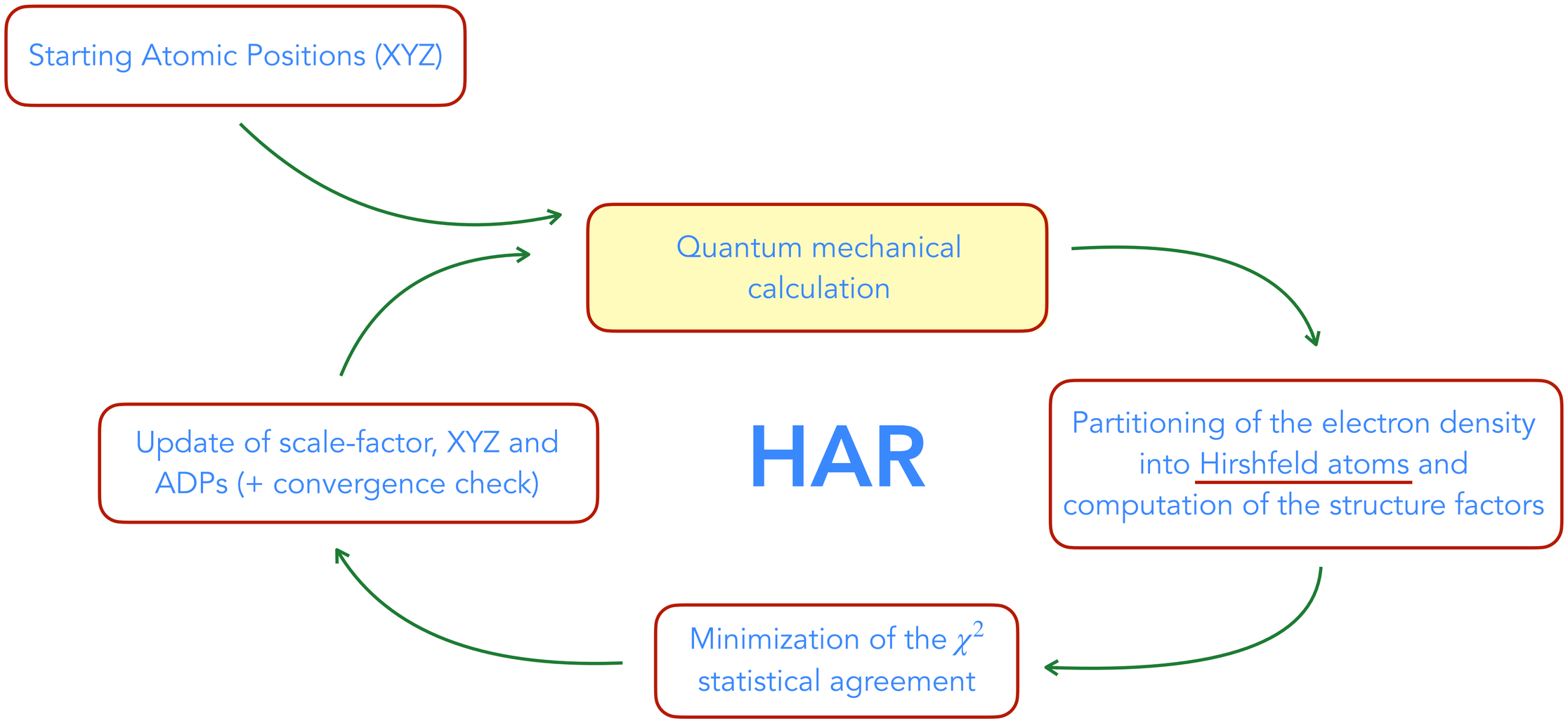

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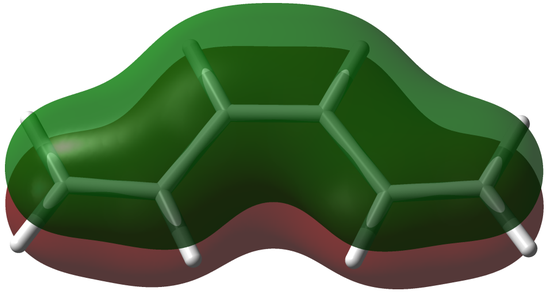
Coupling of HAR with quantum chemistry methods based on Extremely Localized Molecular Orbitals (ELMOs)

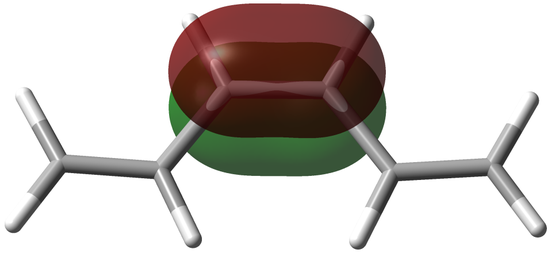
Extremely Localized Molecular Orbitals



Canonical Hartree-Fock
Molecular Orbitals

(completely delocalized orbitals)

≠



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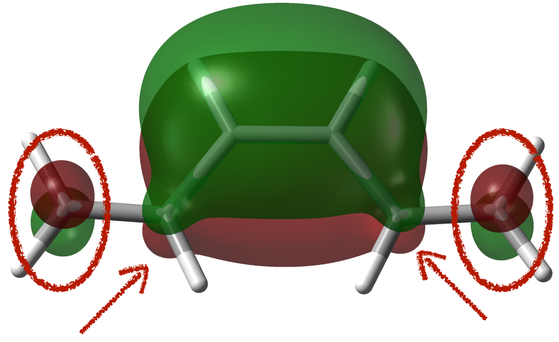

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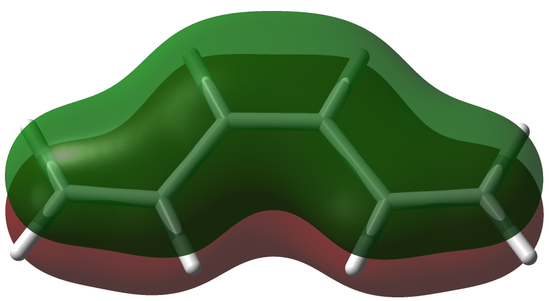

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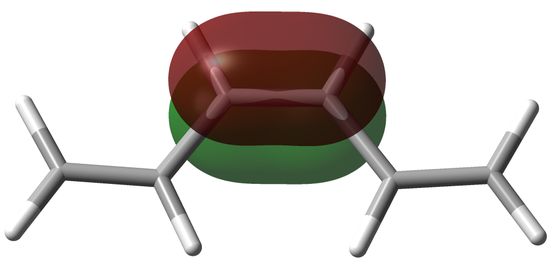

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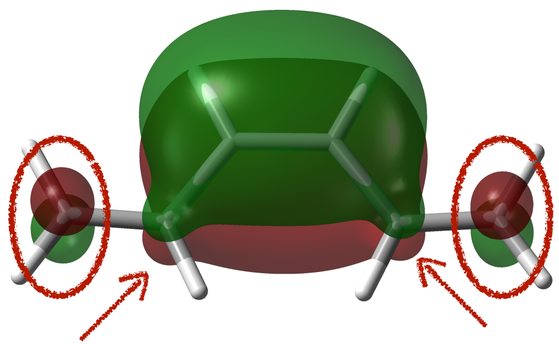

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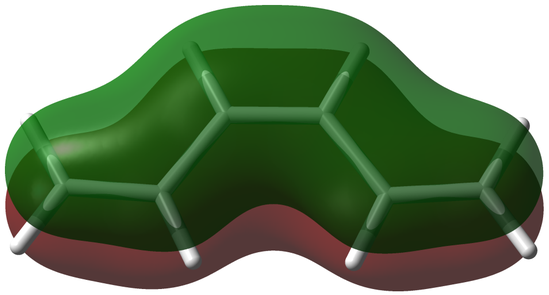

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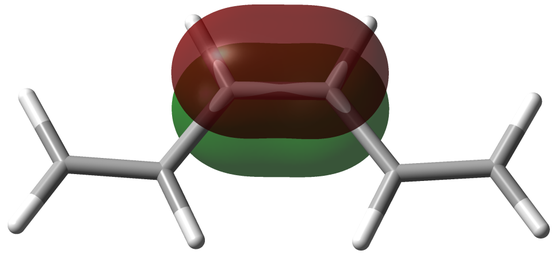

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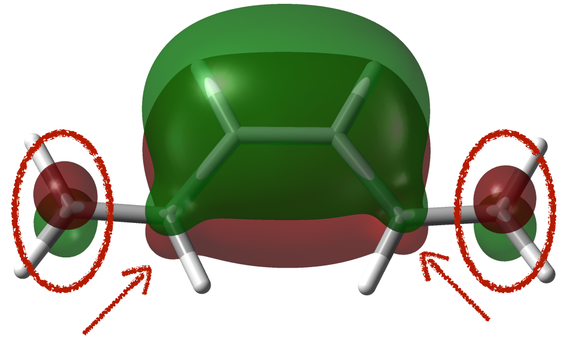

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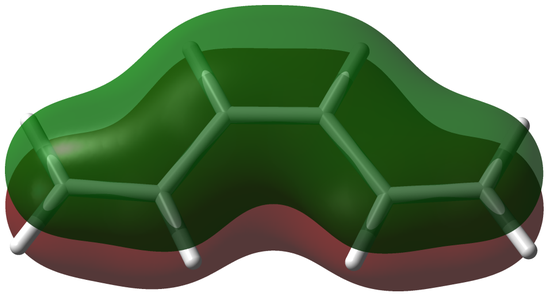
(localized orbitals but with"tails")

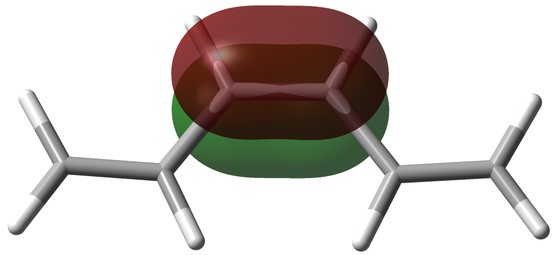
Extremely Localized Molecular Orbitals



Canonical Hartree-Fock
Molecular Orbitals

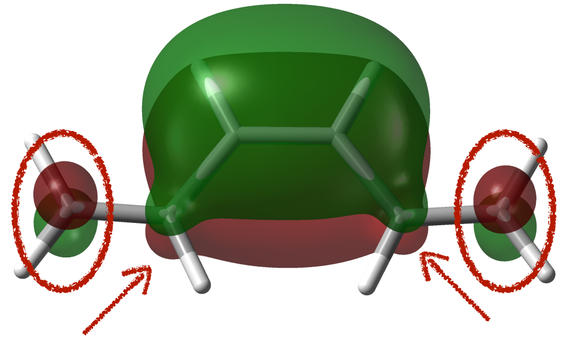
(completely delocalized orbitals)

≠



Extremely Localized Molecular Orbitals
(ELMOs)

≠



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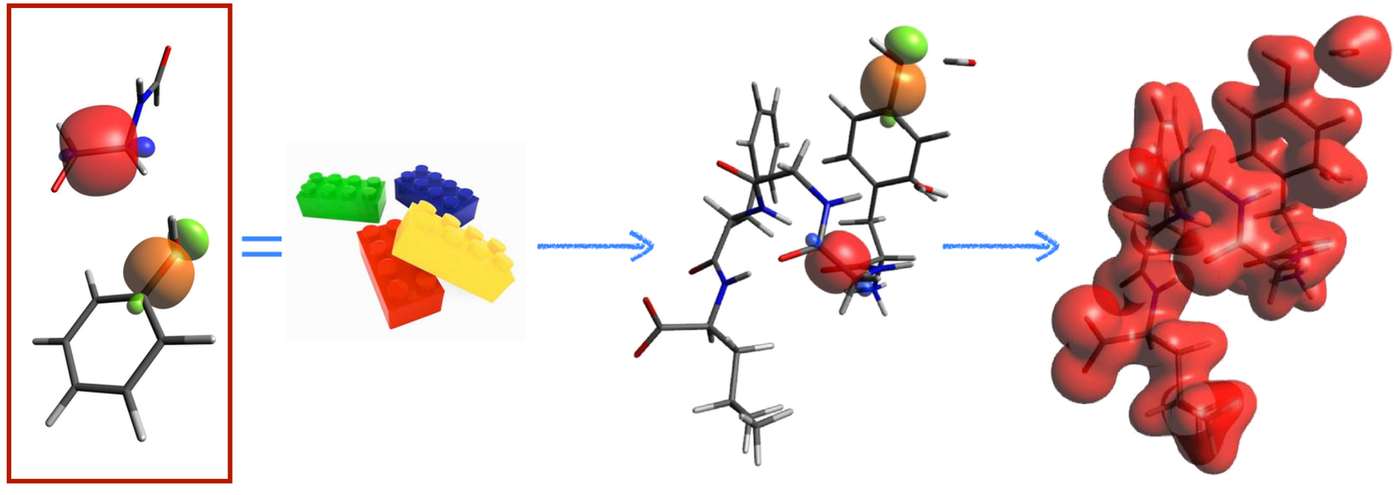
The ELMOs Transferability



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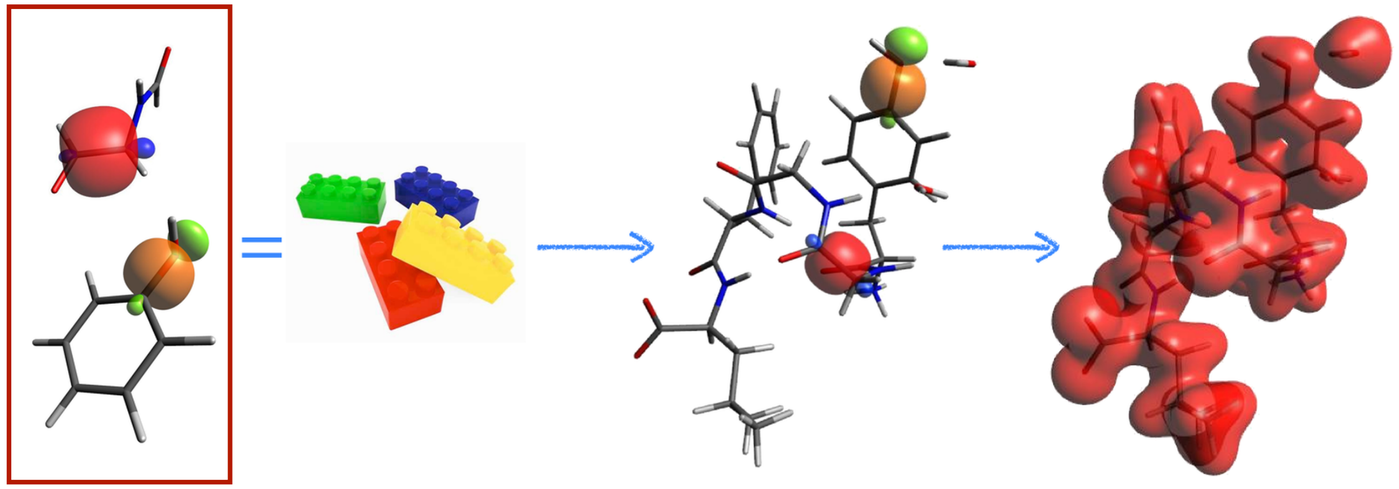

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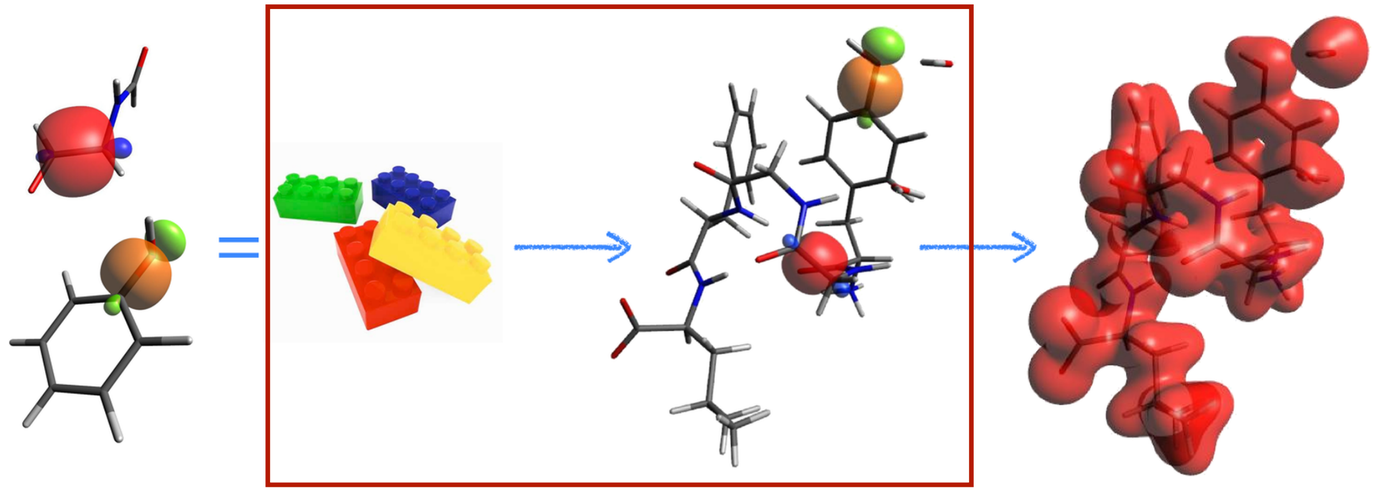

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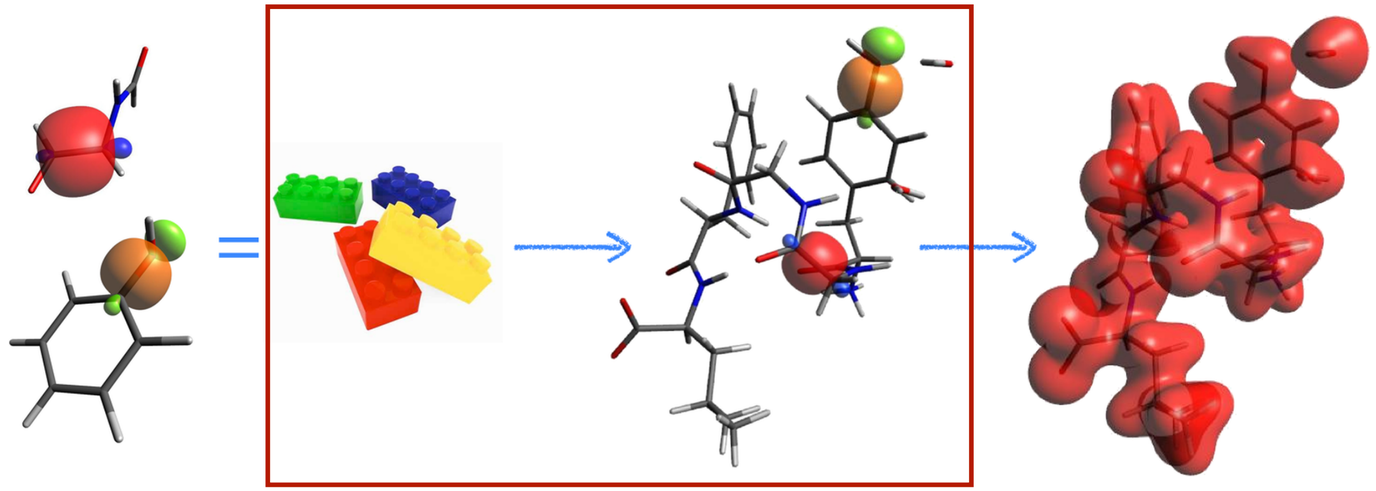

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B. Meyer, B. Guillot, M. F. Ruiz-Lopez, A. Genoni, *J. Chem. Theory Comput.* **12**, 1052 (2016)

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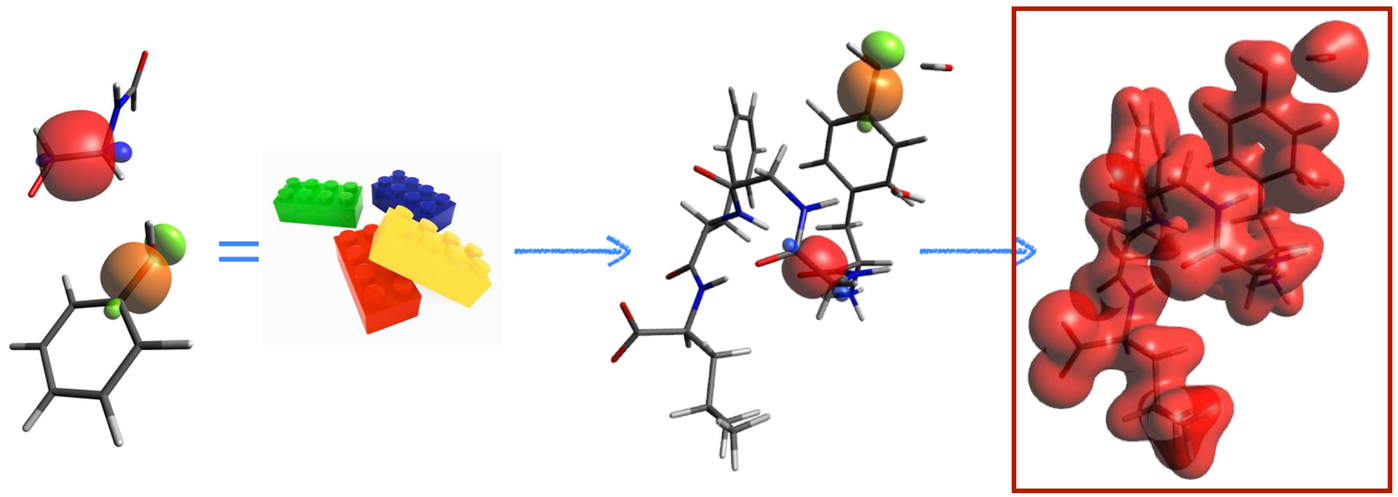

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→ Preliminary investigations on ELMOs transferability →

Assembling ELMO-libraries to reconstruct approximate wavefunctions and electron densities of large molecules (polypeptides and proteins)

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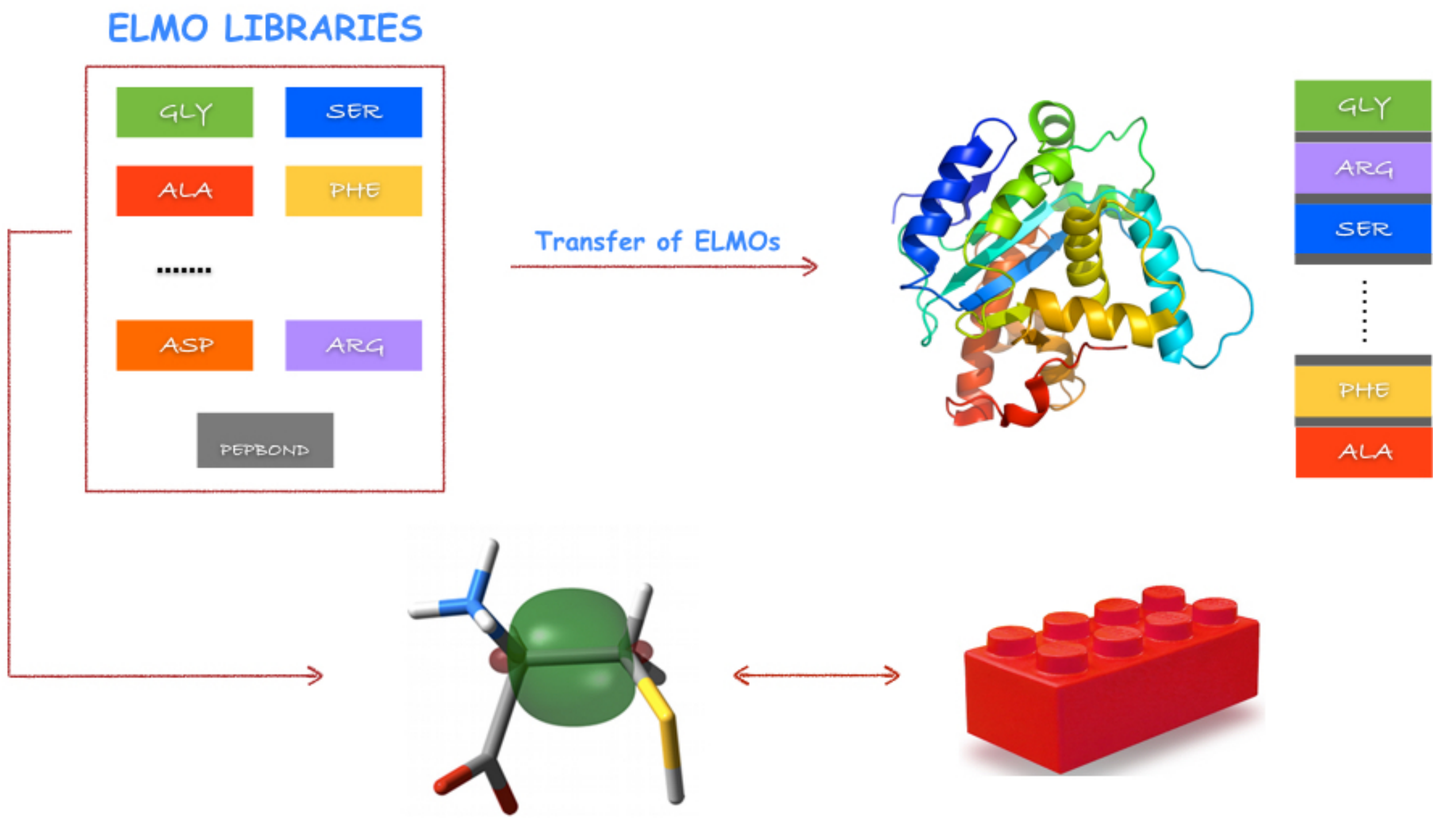
Libraries of Extremely Localized Molecular Orbitals



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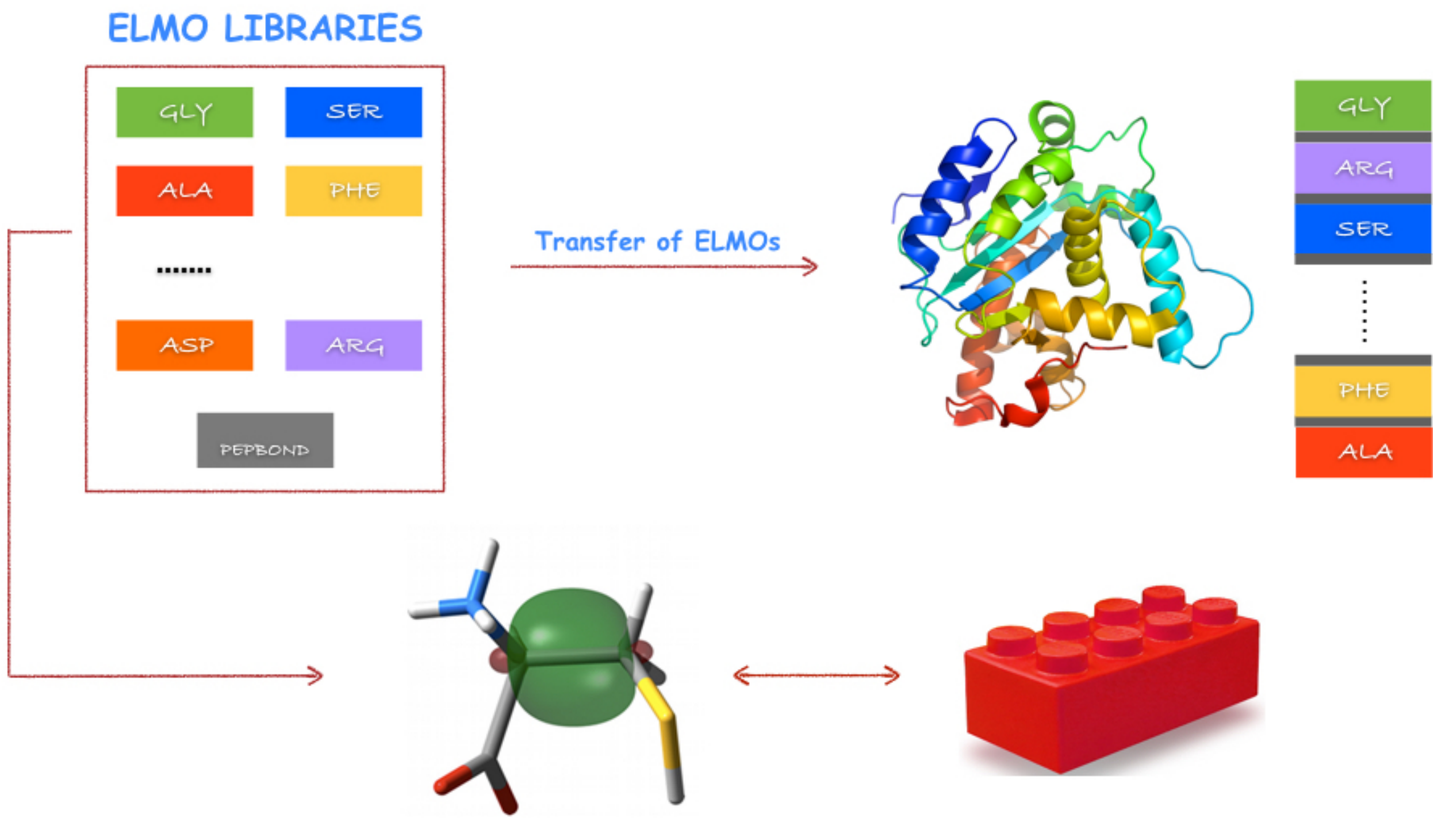

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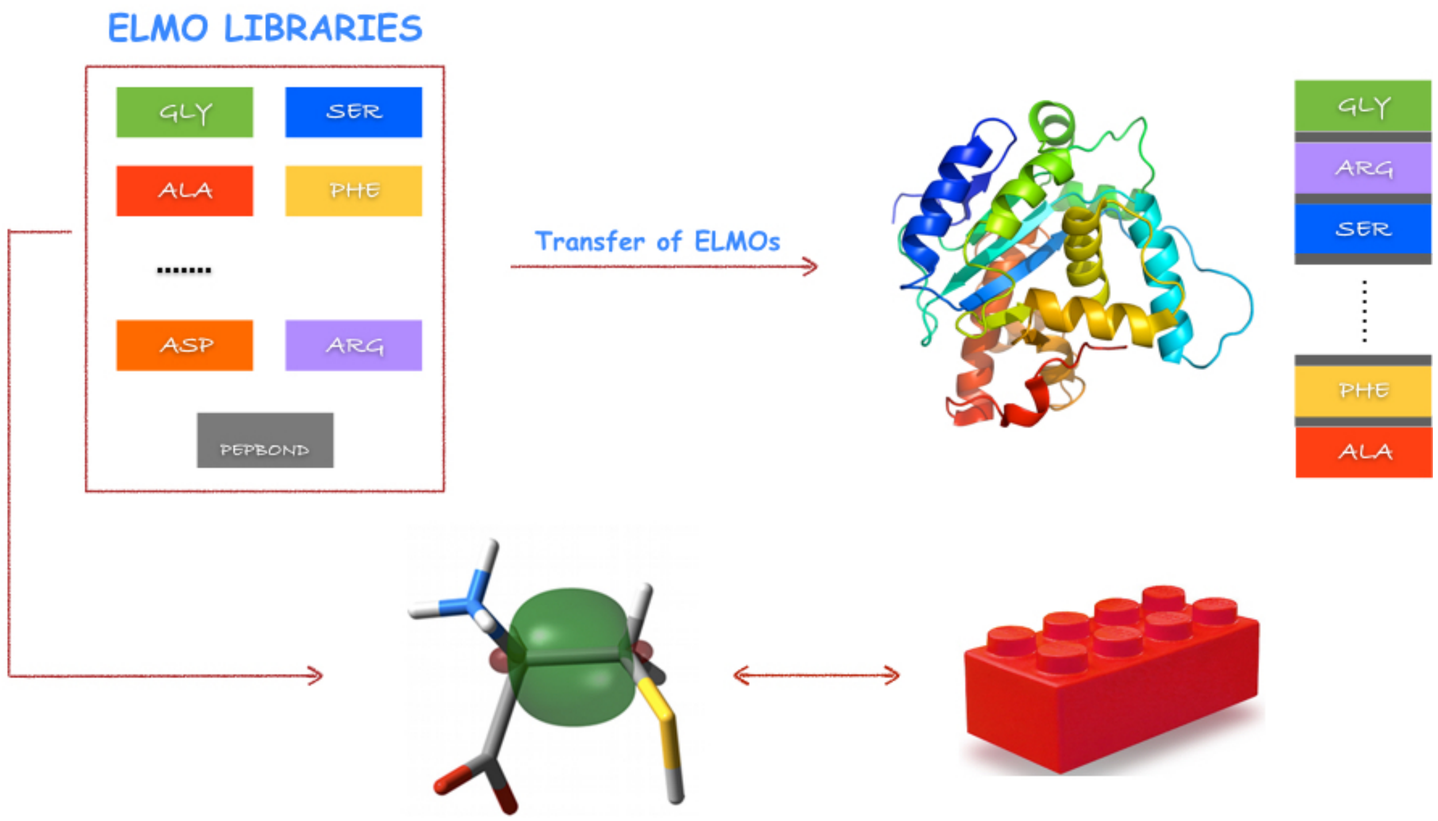

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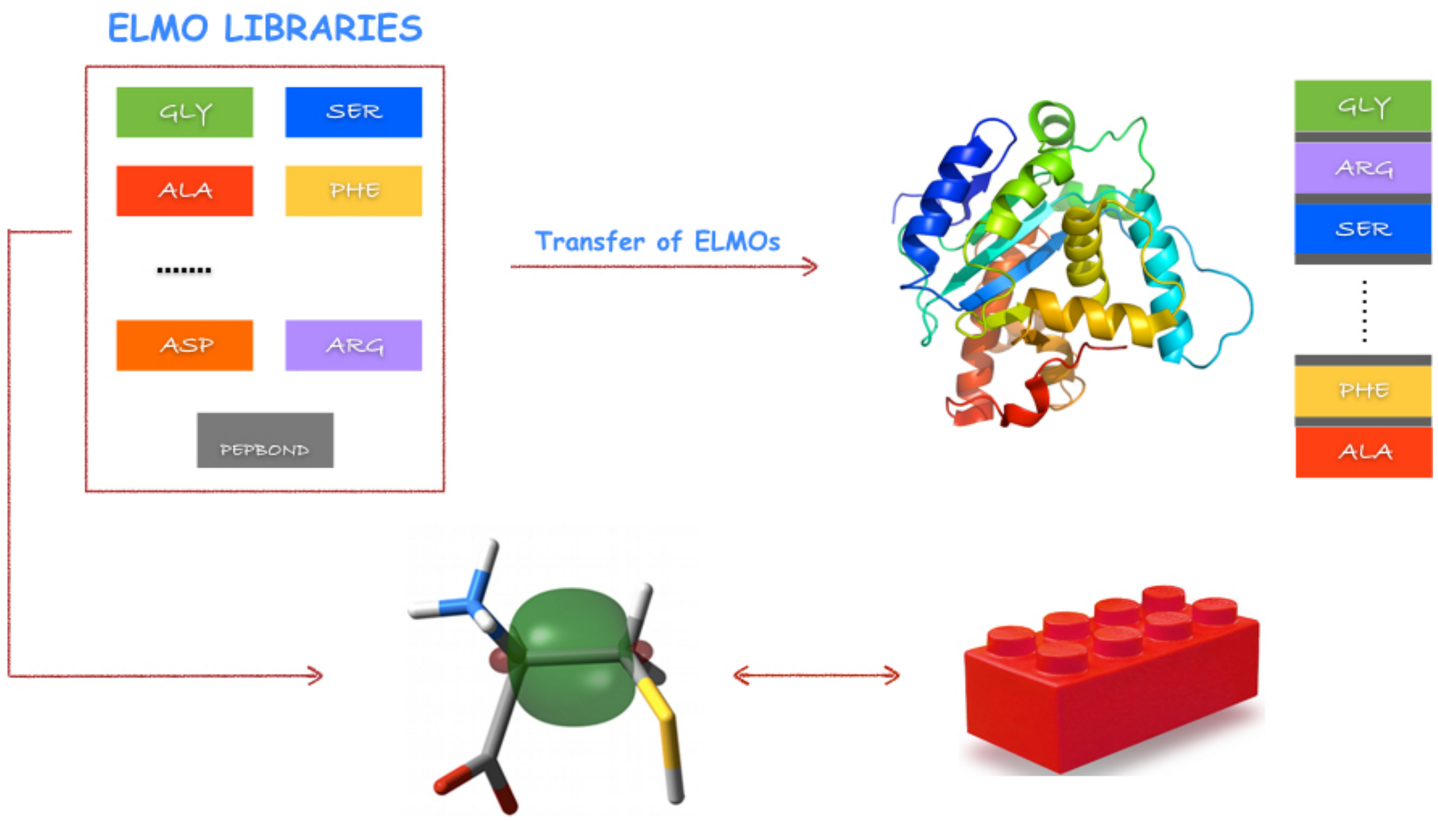

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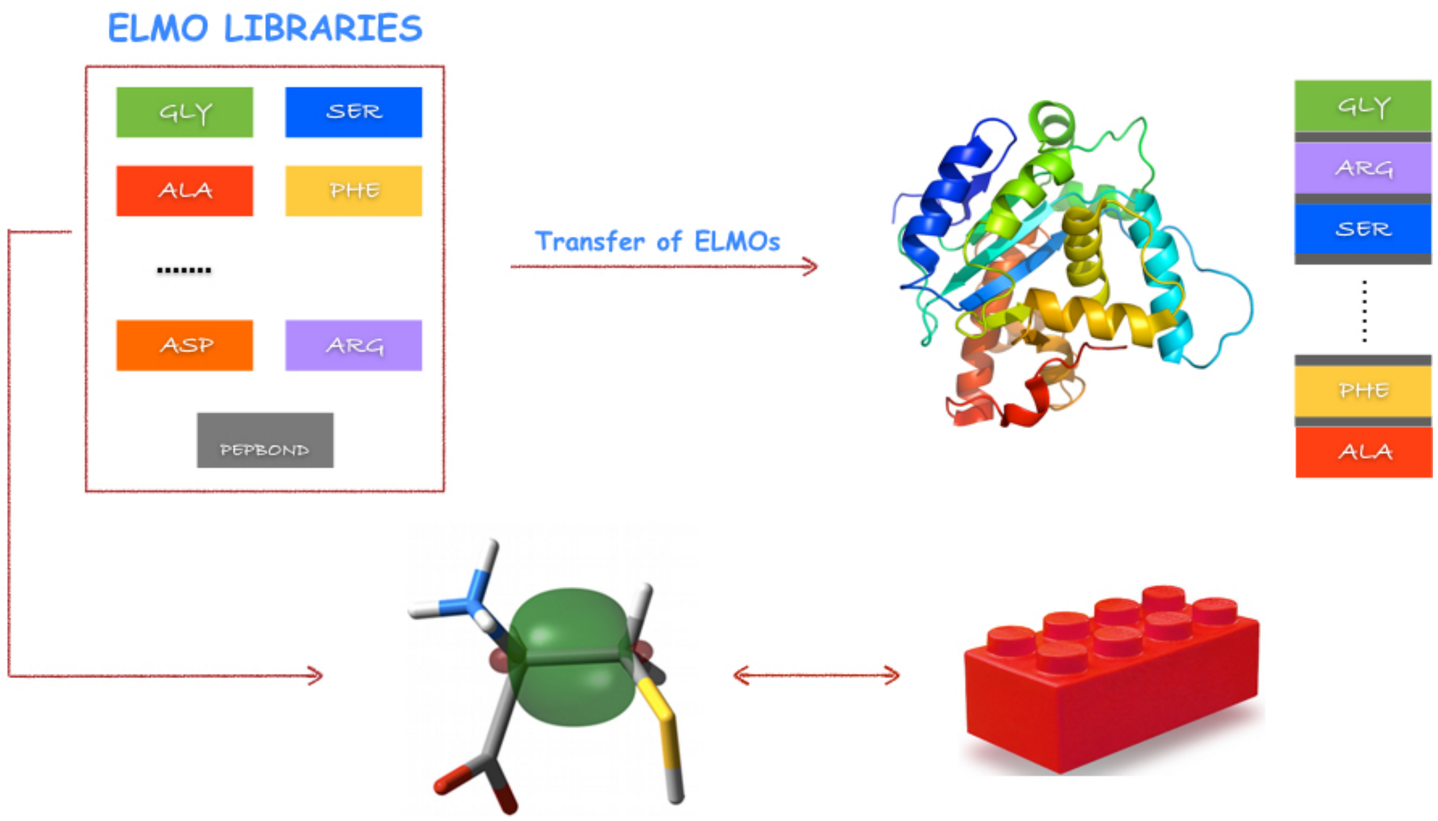

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B. Meyer, A. Genoni, *J. Phys. Chem. A* **122**, 8965 (2018)

ELMO Libraries: Application to a Protein

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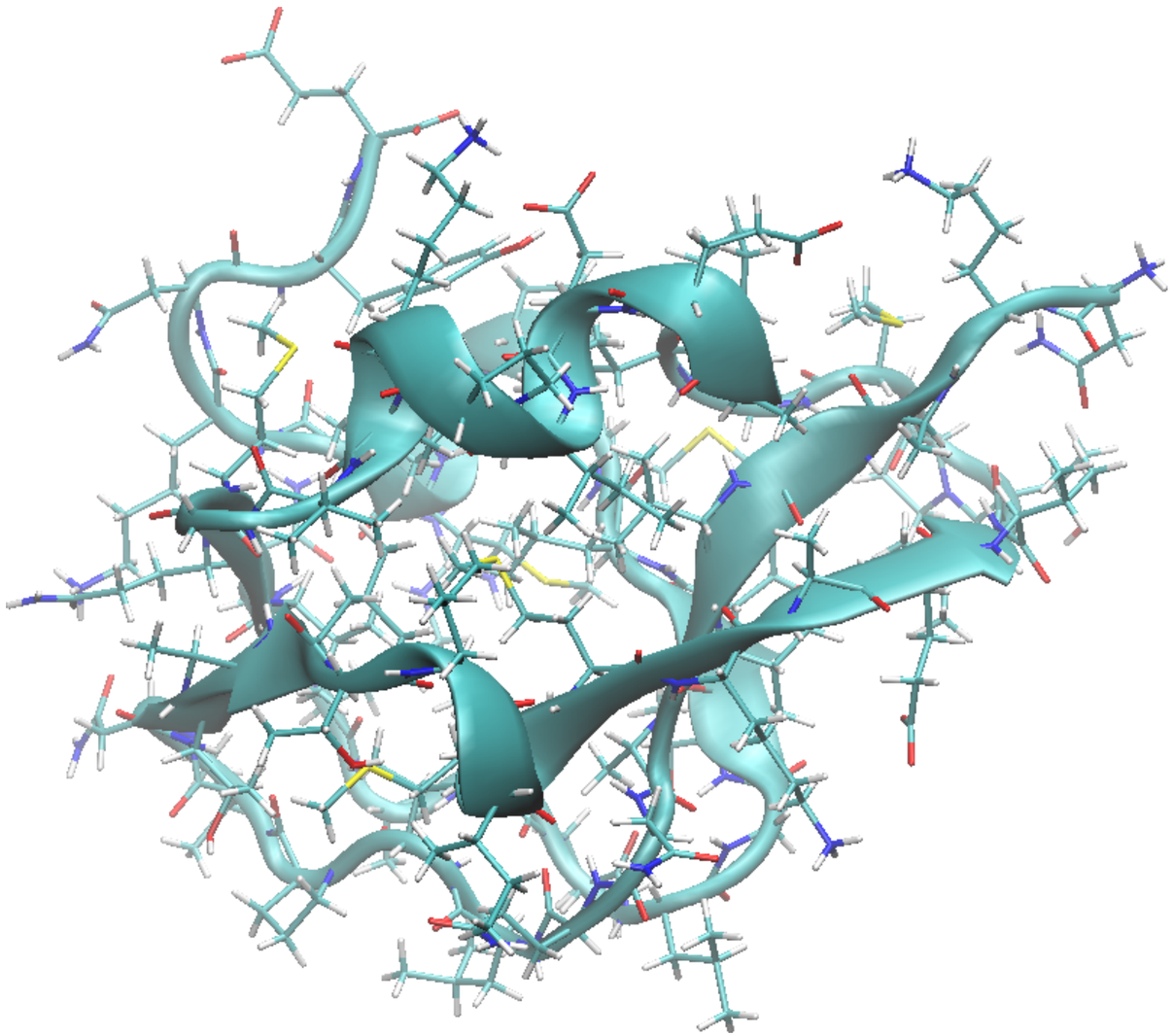
ELMO Libraries: Application to a Protein

Antifreeze Protein RD1 (PDB Code: 1UCS, 64 residues, 997 atoms)



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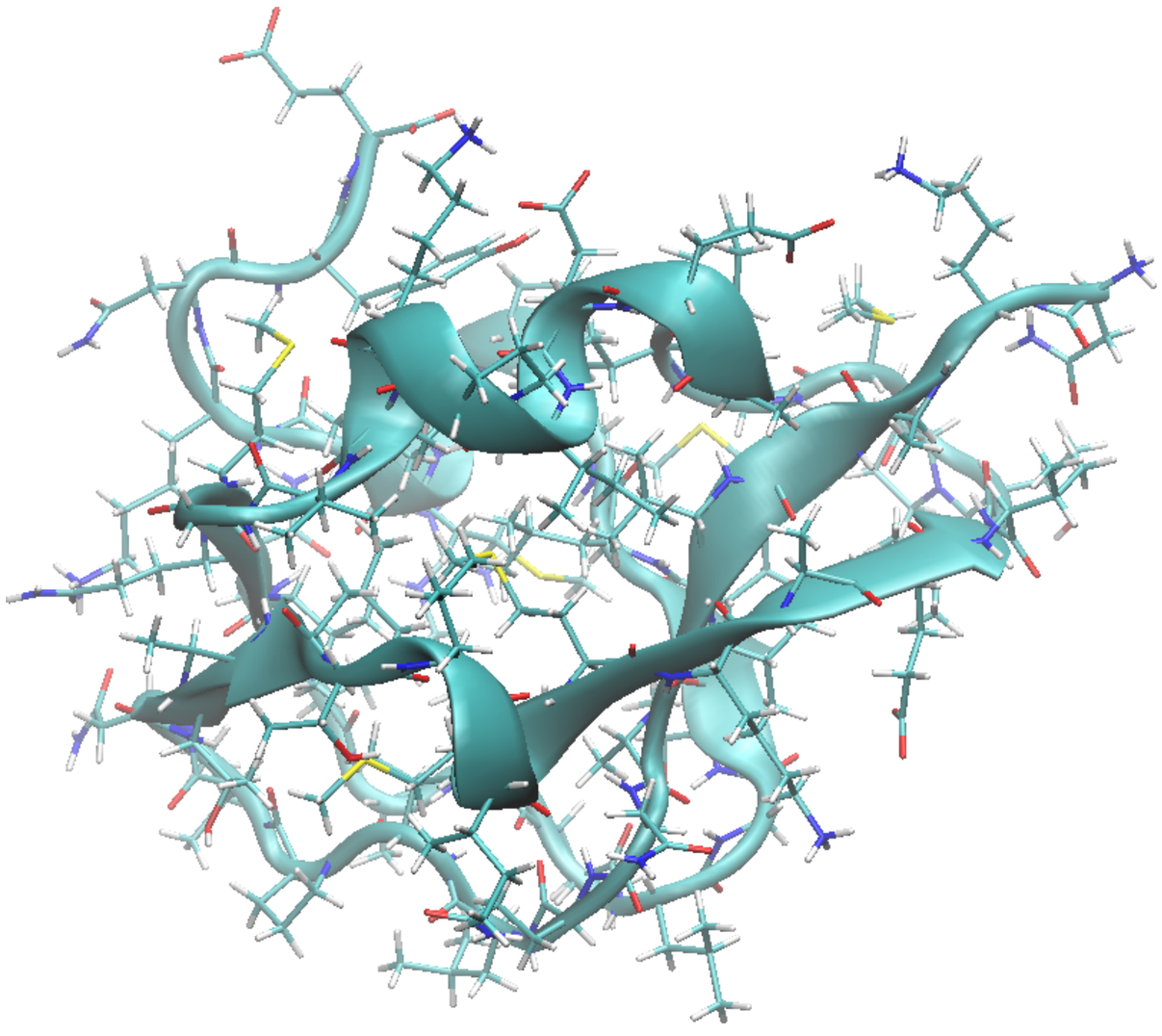

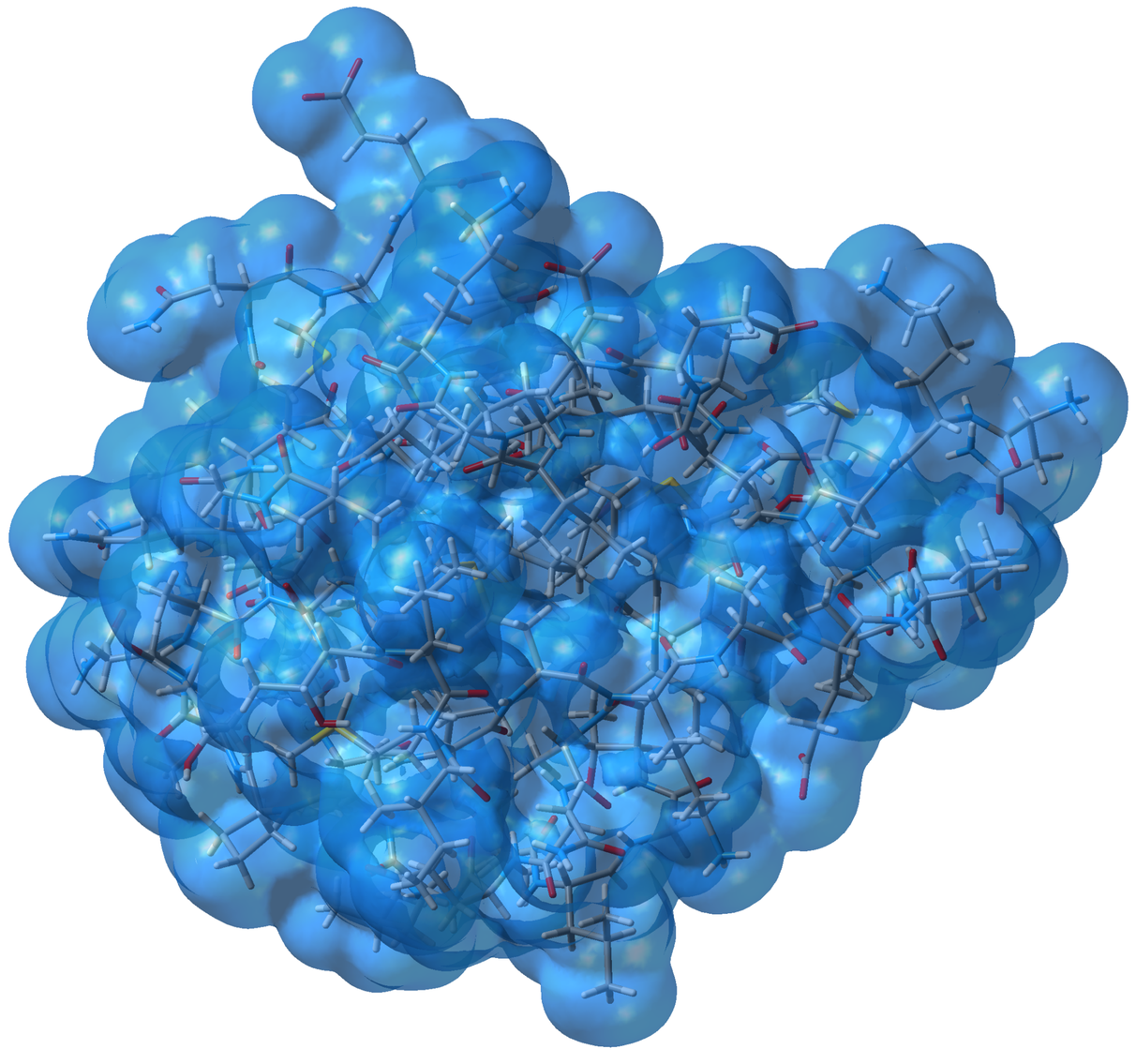

ELMO Electron Density (0.001 e/bohr^3 isosurface)

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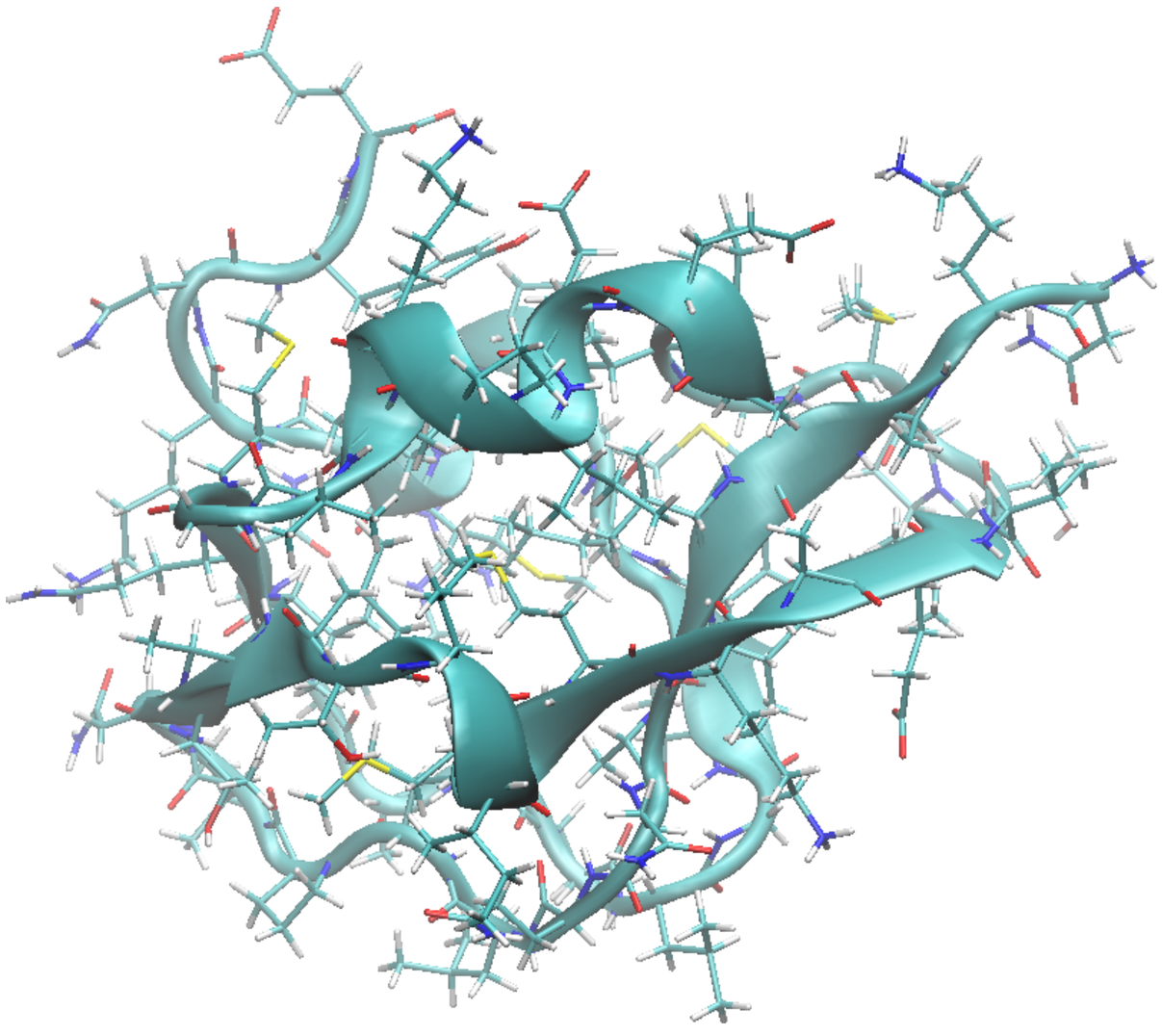
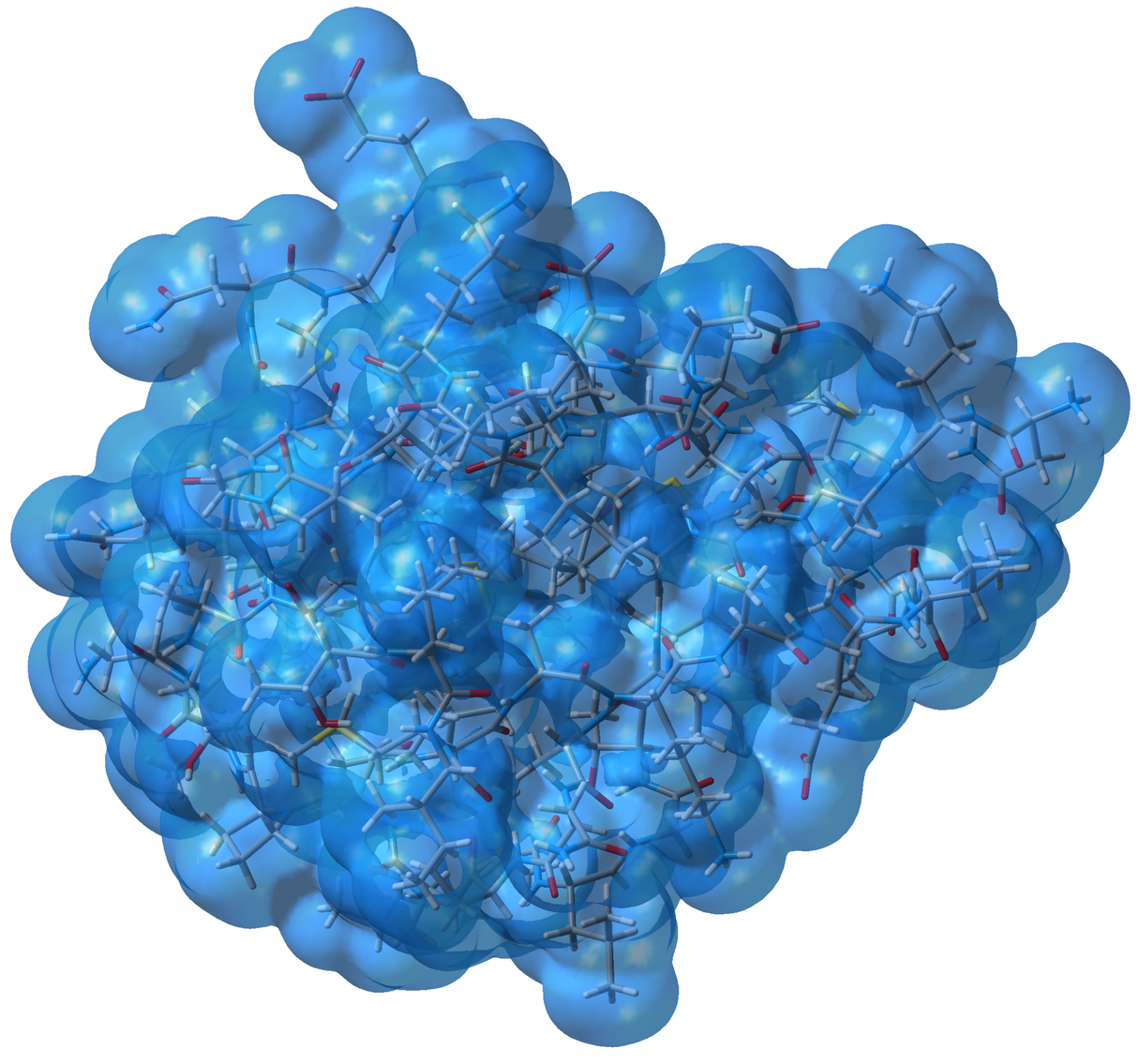


Global CPU time with 6-311G** basis-set:
~**2.5 minutes** Vs. ~ **10 days** for Hartree-Fock calculation



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QM/ELMO Embedding Method

ELMOs and ELMO libraries were the bases for the development of a new multi-scale embedding method:

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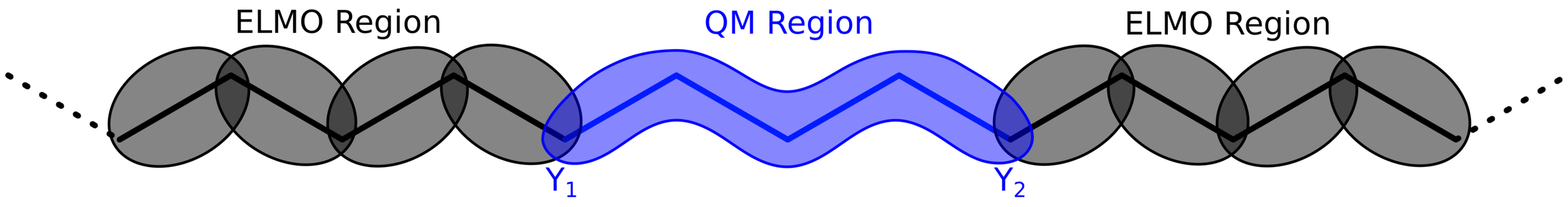

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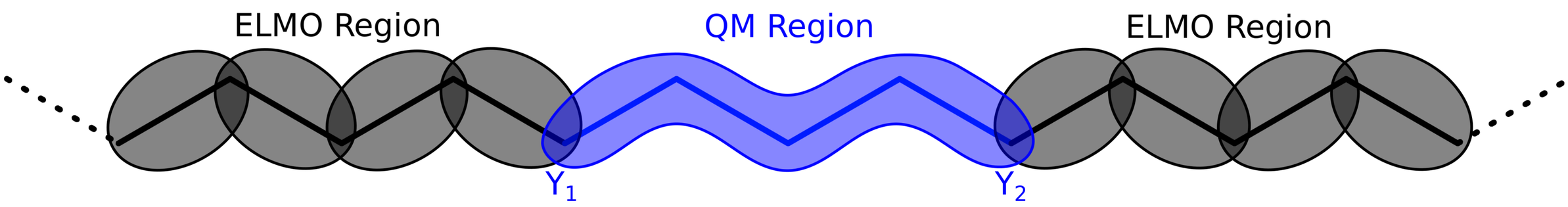

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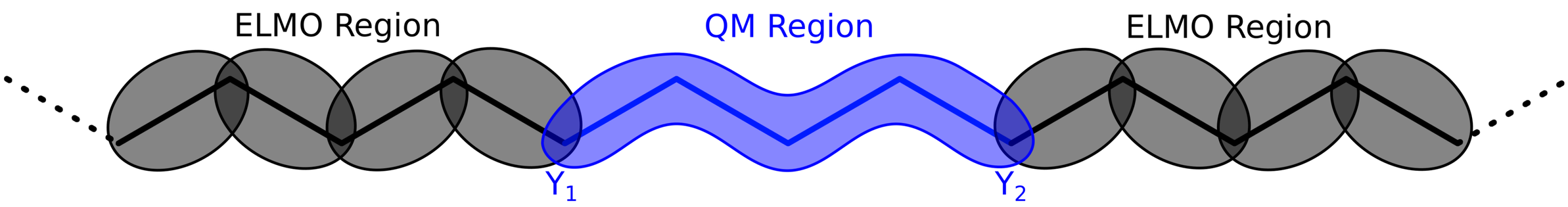

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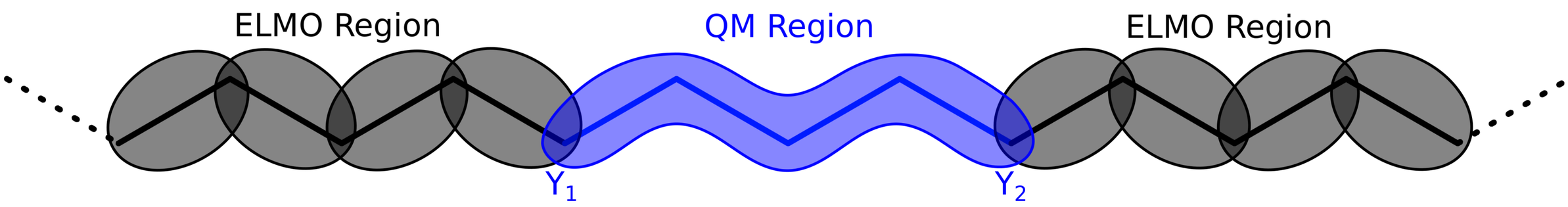

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- Initially developed in the framework of the restricted Hartree-Fock formalism
- Extended to other ground state methods: DFT, post-Hartree-Fock techniques (MP2, Coupled Cluster, etc.)
- Combined with strategies for excited states: Time-Dependent DFT, Equation-of-Motion Coupled Cluster and IMOM
- More recently generalized to QM/ELMO/MM (outermost layer treated at molecular mechanics level)

G. Macetti, A. Genoni, *J. Phys. Chem. A* **123**, 9420 (2019)

G. Macetti, E. K. Wieduwilt, X. Assfeld, A. Genoni, *J. Chem. Theory Comput.* **16**, 3578 (2020)

G. Macetti, A. Genoni, *J. Chem. Theory Comput.* **16**, 7490 (2020)

G. Macetti, E. K. Wieduwilt, A. Genoni, *J. Phys. Chem. A* **125**, 2709 (2021)

G. Macetti, A. Genoni, *J. Chem. Theory Comput.* **17**, 4169 (2021)

G. Macetti, A. Genoni, *J. Phys. Chem. A* **125**, 6013 (2021)

Larger Computational Cost of HAR

The computational cost of HAR increases with the size of the system under exam

↓

In its original version, HAR cannot be straightforwardly applied to macromolecules

We need QM methods that provide almost instantaneously wavefunctions and electron densities of very large systems

↓

Coupling of HAR with quantum chemistry methods based on Extremely Localized Molecular Orbitals (ELMOs)

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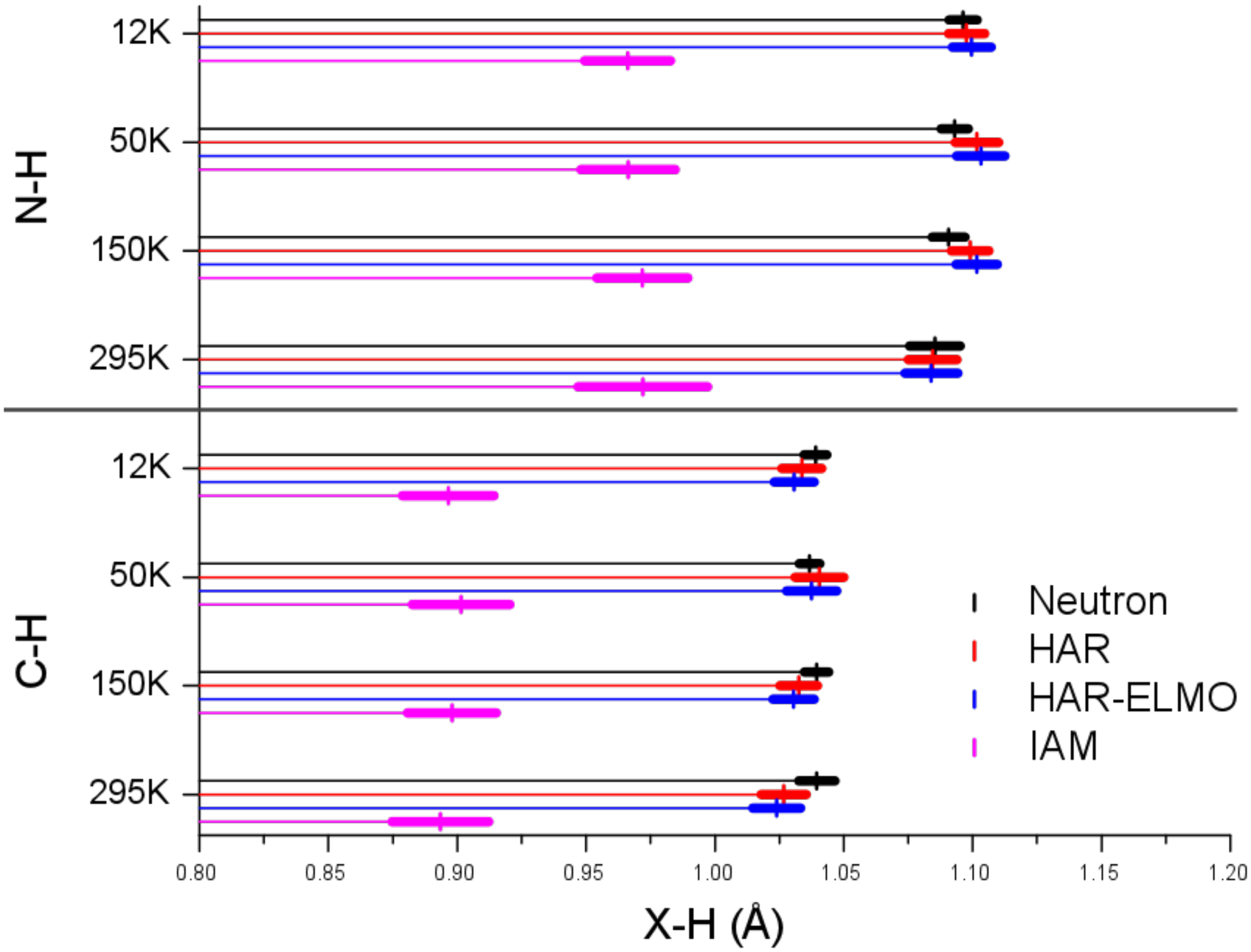
Coupling of HAR with ELMO libraries and QM/ELMO approach

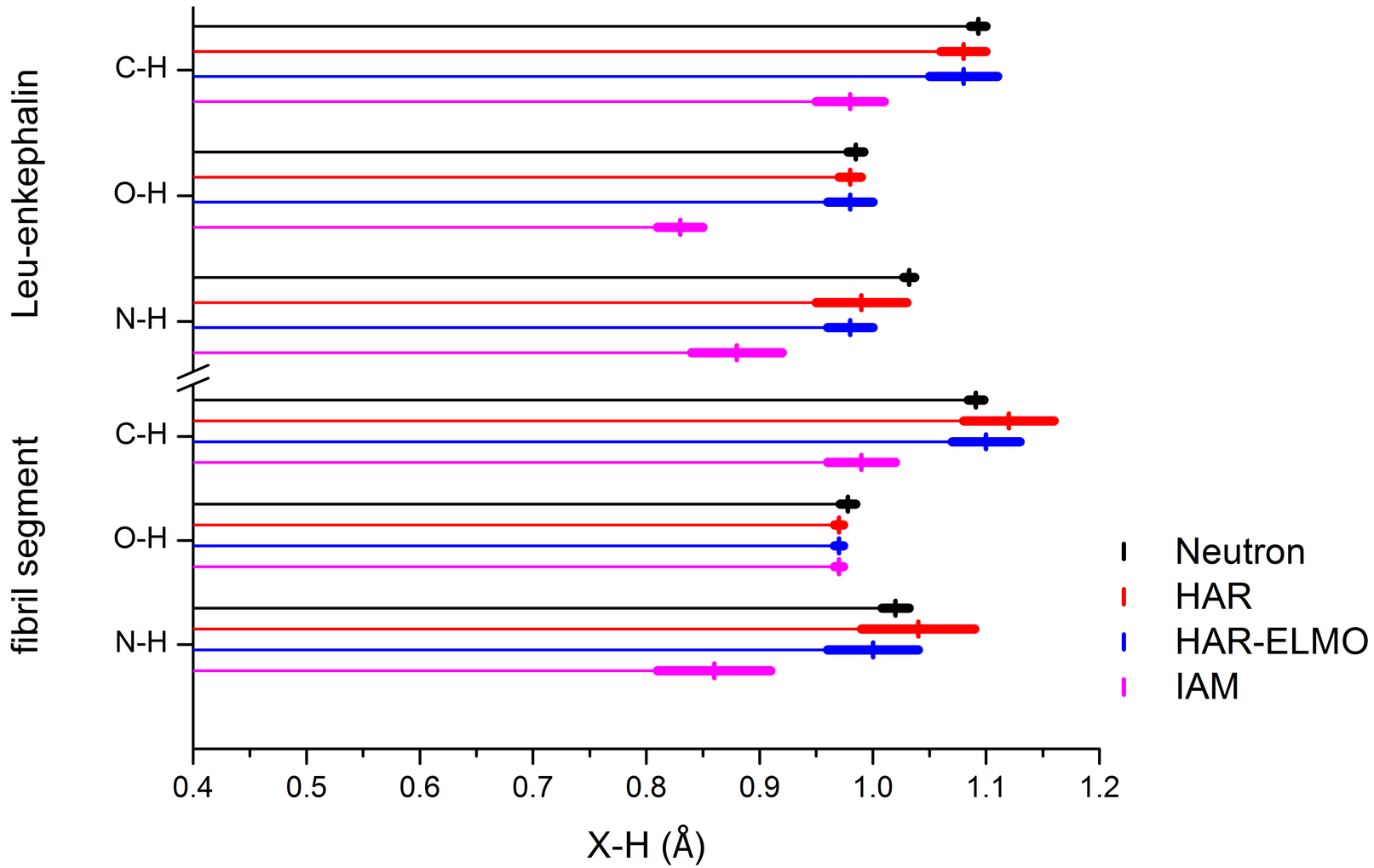
HAR-ELMO: Validation Tests on Gly-*L*-Ala



L. A. Malaspina, E. K. Wieduwilt,…, S. Grabowsky, A. Genoni, *J. Phys. Chem. Lett.* 10, 6973 (2019)

HAR-ELMO: Application to Polypeptides

General statistics for E-H bond-lengths



Neutron reference values = Allen & Bruno average values

L. A. Malaspina, E. K. Wieduwilt,…, S. Grabowsky, A. Genoni, *J. Phys. Chem. Lett.* 10, 6973 (2019)

HAR-ELMO: Application to the Protein Crambin

Two different X-ray data sets have been considered for crambin: 0.54 Å and 0.73 Å

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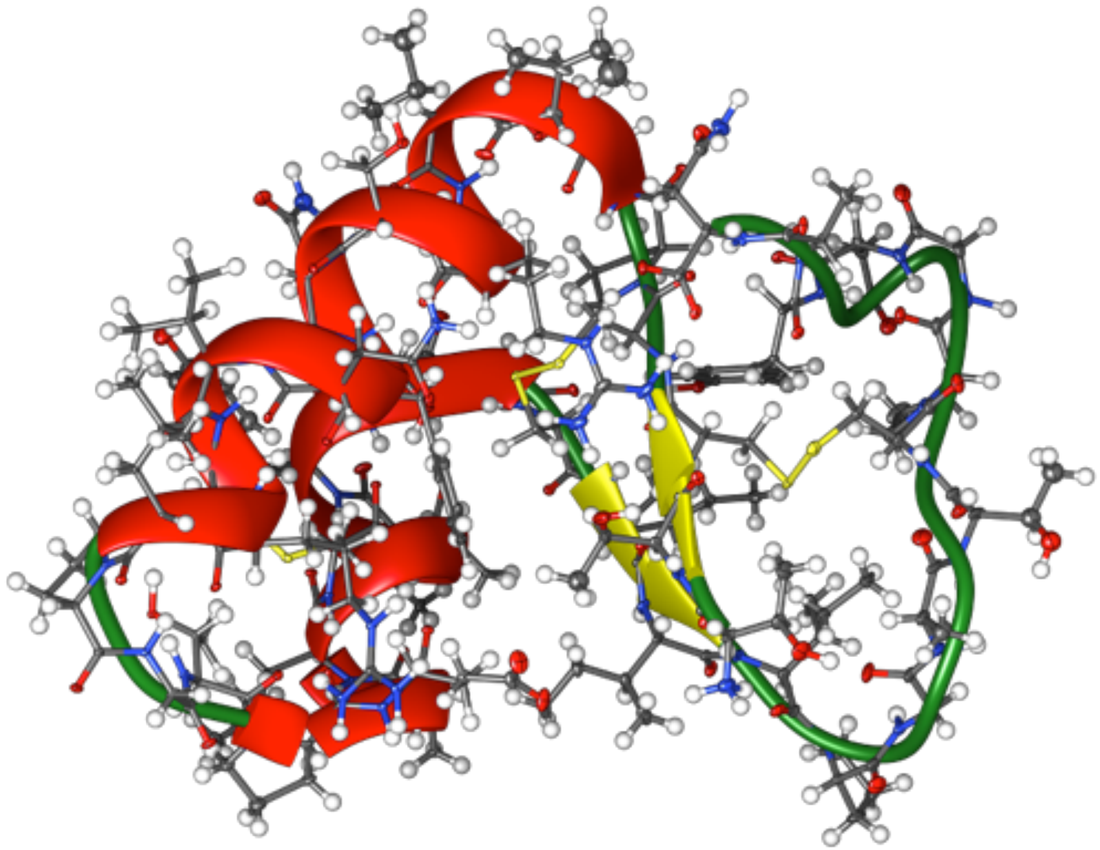

HAR-ELMO REFINED STRUCTURE OF CRAMBIN

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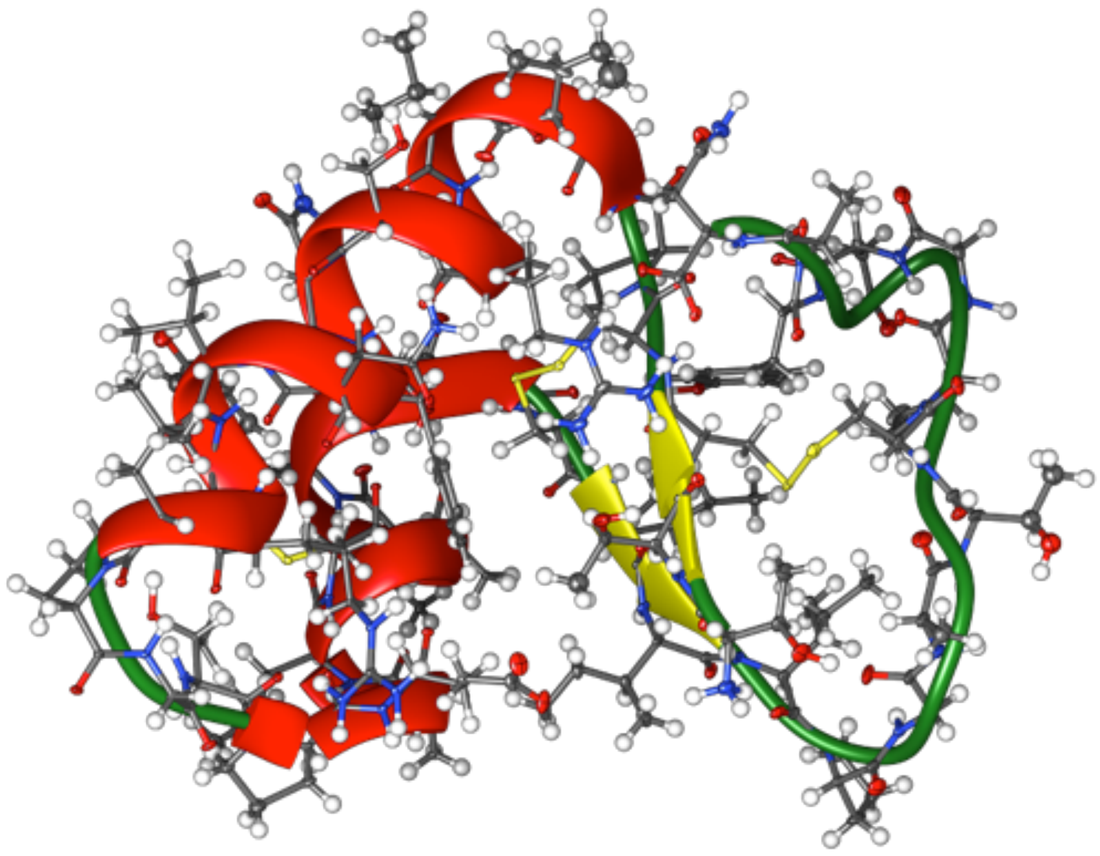

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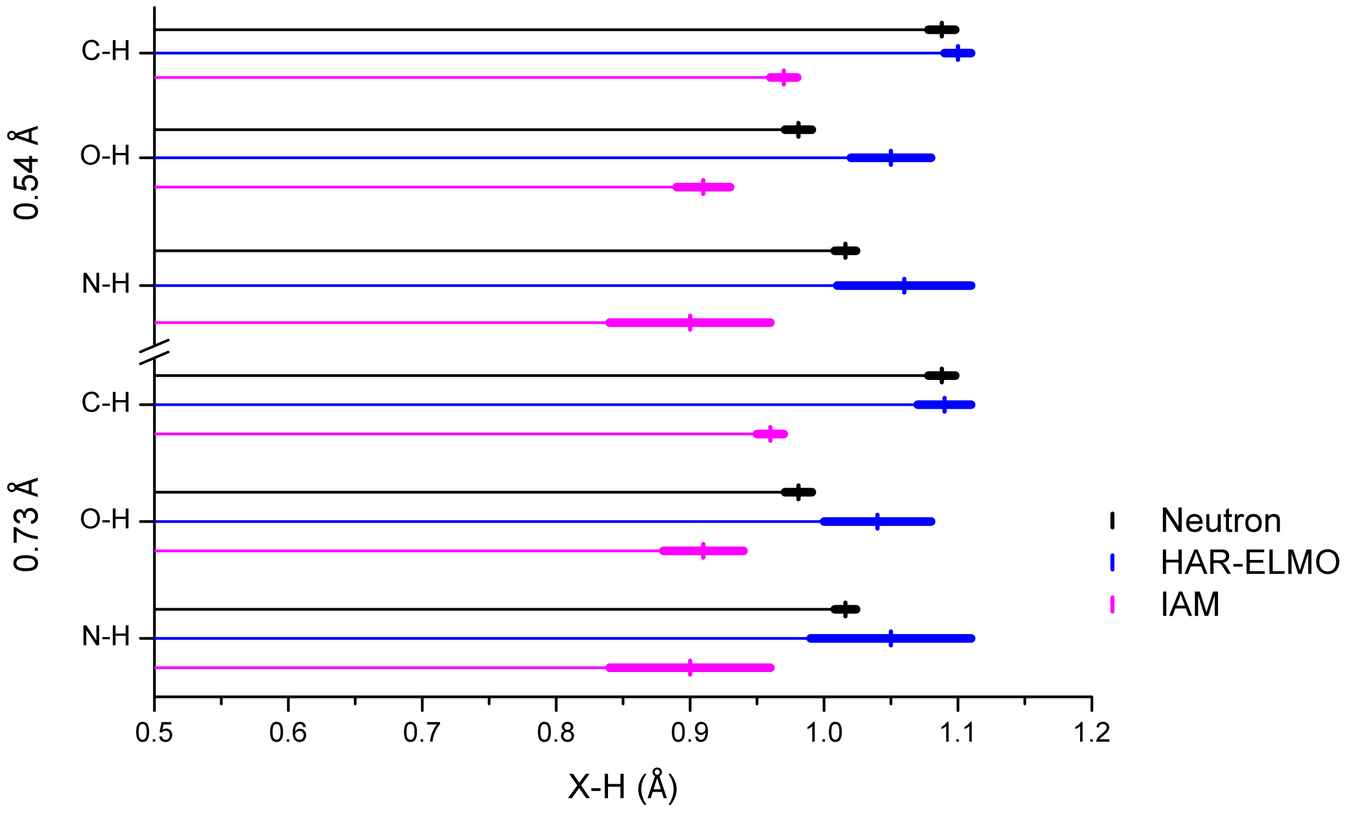

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HAR-ELMO: Computational Cost

System	CPU TIME (days:hours:min:s)	
	HAR-HF	HAR-ELMO
Leu-Enkephalin	0:9:52:00	0:1:44:17
Fibril-forming segment	1:7:00:00	0:0:22:56
Crambin (0.54 Å)	IMPOSSIBLE	9:23:47:53
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HAR-ELMO ALLOWS QUANTUM CRYSTALLOGRAPHIC REFINEMENTS WHEN THE APPLICATION OF THE TRADITIONAL HAR-HF METHOD IS IMPOSSIBLE/IMPRACTICAL

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From HAR-ELMO to HAR-QM/ELMO

HAR-ELMO already provides quite successful results for the determination of hydrogen atom positions
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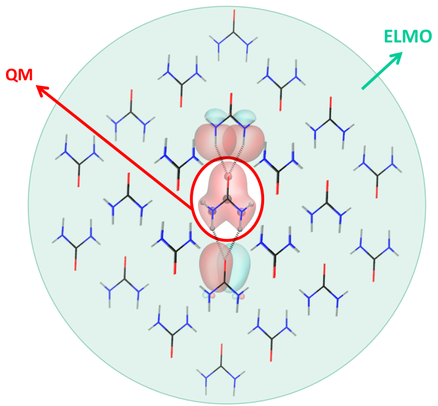
QM/ELMO already coupled with HAR in a different way → Accurate refinements of small molecule crystal structures

The HAR-QM/ELMO Method

HAR-QM/ELMO method to refine crystal structures characterized by strong intermolecular interactions

(traditional strategy of using surrounding point charges and dipoles is not enough)



QM/ELMO strategy for the quantum chemical calculations of HAR with:

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The HAR-QM/ELMO Method

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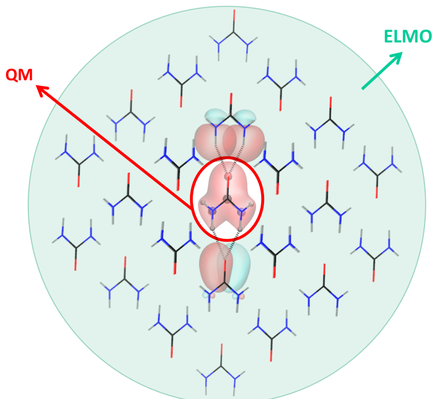

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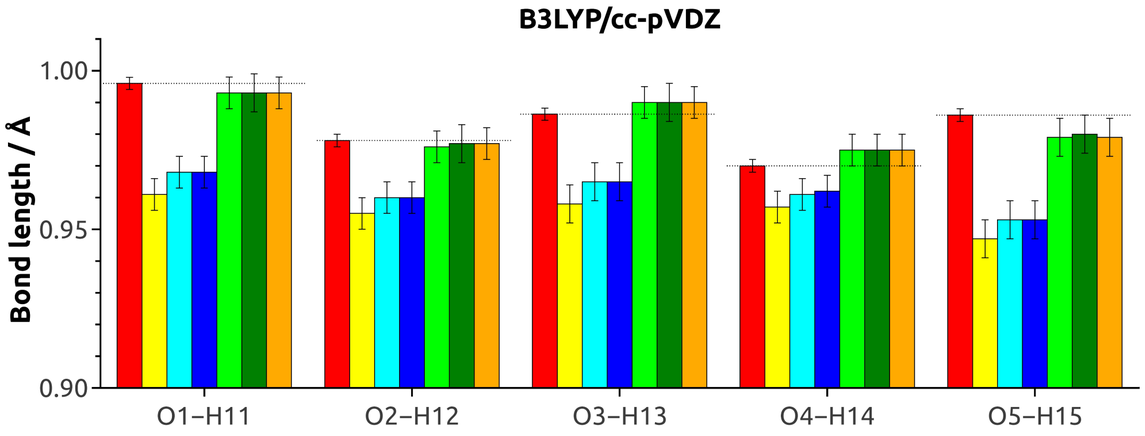
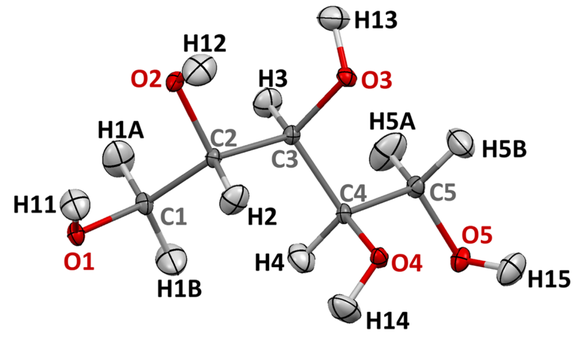
Application to the refinement of the xylitol crystal structure (network of strong hydrogen bonds)





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Concluding Remarks

Methods with a strong interplay between quantum chemistry and X-ray diffraction measurements

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Methods with a strong interplay between quantum chemistry and X-ray diffraction measurements

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Quantum chemistry calculations and quantum chemistry methods can be exploited to improve the results of traditional crystallographic structural refinements

Quantum Chemistry and (Quantum) Crystallography are strongly related and may “contaminate” each other to obtain better results and to develop more and more advanced methods in both fields

Acknowledgments

Funding:

Acknowledgments

Funding:

anr agence nationale de la recherche
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… and thanks for your attention !

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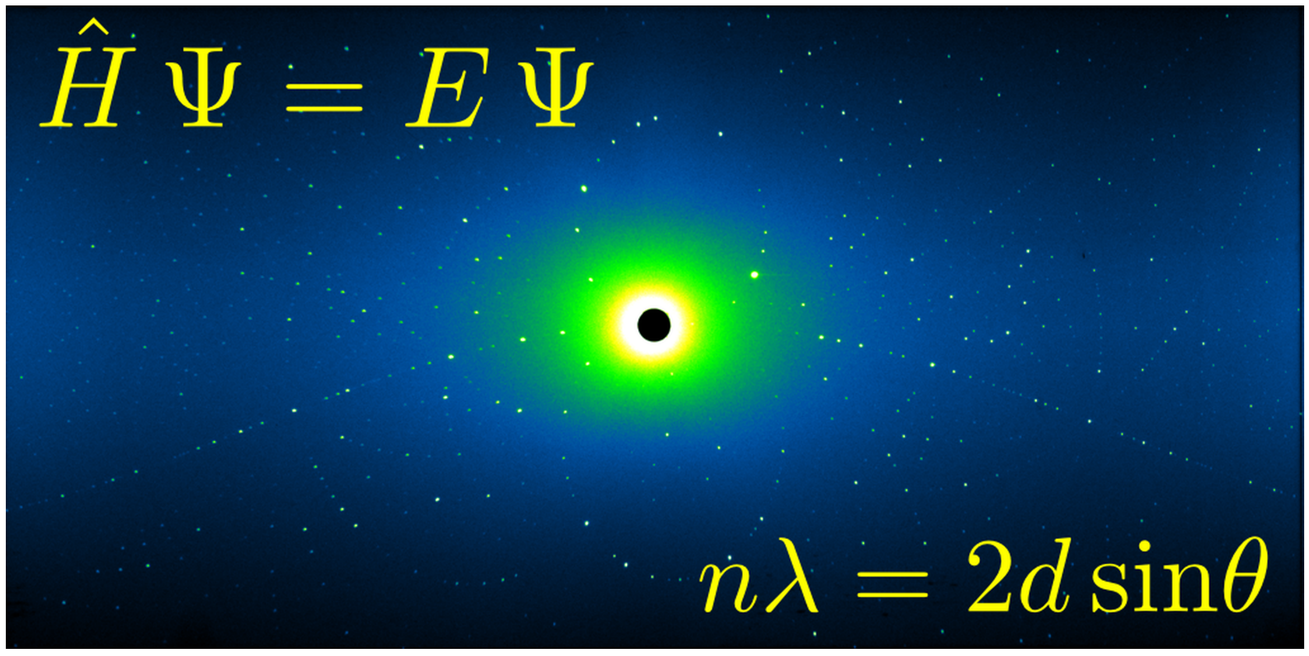
About the Connections and Possible Contaminations between Quantum Chemistry and Quantum Crystallography



3rd Quantum International Frontier - QIF3
Łódź, Poland - June 24, 2023