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OMICS Group International is an amalgamation of Open Access publications and worldwide international science conferences and events. Established in the year 2007 with the sole aim of making the information on Sciences and technology ‘Open Access’, OMICS Group publishes 400 online open access scholarly journals in all aspects of Science, Engineering, Management and Technology journals. OMICS Group has been instrumental in taking the knowledge on Science & technology to the doorsteps of ordinary men and women. Research Scholars, Students, Libraries, Educational Institutions, Research centers and the industry are main stakeholders that benefitted greatly from this knowledge dissemination. OMICS Group also organizes 300 International conferences annually across the globe, where knowledge transfer takes place through debates, round table discussions, poster presentations, workshops, symposia and exhibitions.

About OMICS Group Conferences

OMICS Group International is a pioneer and leading science event organizer, which publishes around 400 open access journals and conducts over 300 Medical, Clinical, Engineering, Life Sciences, Phrama scientific conferences all over the globe annually with the support of more than 1000 scientific associations and 30,000 editorial board members and 3.5 million followers to its credit.

OMICS Group has organized 500 conferences, workshops and national symposiums across the major cities including San Francisco, Las Vegas, San Antonio, Omaha, Orlando, Raleigh, Santa Clara, Chicago, Philadelphia, Baltimore, United Kingdom, Valencia, Dubai, Beijing, Hyderabad, Bengaluru and Mumbai.

Zur Anzeige wird der QuickTime™ Dekompressor „“ benötigt.

3rd International Conference and Exhibition on

Materials Science & Engineering

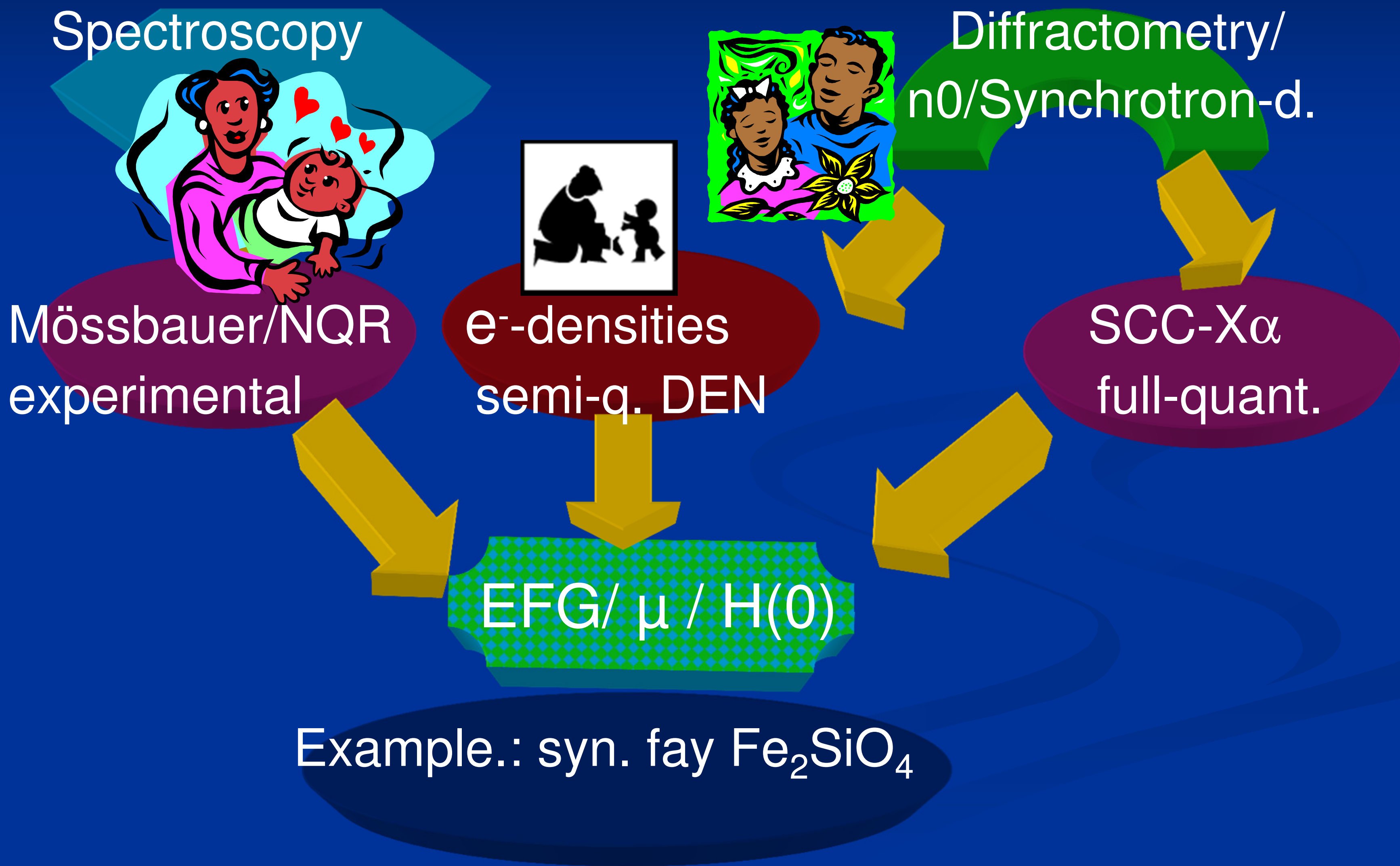
October 06-08, 2014 San Antonio, USA

Application of a Difference Electron Nanoscope (DEN) - correlation between 3D magnetical structures of synthetic fayalite with synchrotron and neutron diffraction and Mössbauer spectroscopy

Lottermoser W, Steiner K, Grodzicki M, Kirfel A, Amthauer G

Dep. of Materials Engineering and Physics/Univ. of Salzburg

Scheme


Spectroscopy
Diffractometry/
n0/Synchrotron-d.
Mössbauer/NQR
experimental
e⁻-densities
semi-q. DEN
SCC-Xα
full-quant.
EFG/ μ / H(0)
Example.: syn. fay Fe_2SiO_4

The electric field gradient (EFG)

- EFG = $\nabla E = -\nabla\nabla V = -\begin{pmatrix} V_{xx} & V_{xy} & V_{xz} \\ V_{yx} & V_{yy} & V_{yz} \\ V_{zx} & V_{zy} & V_{zz} \end{pmatrix}$

...with $V_{ij} = \partial^2 V / \partial i\, \partial j$ (i,j = x,y,z)

- Choice of the main axes components:

  $|V_{zz}| \geq |V_{yy}| \geq |V_{xx}|$

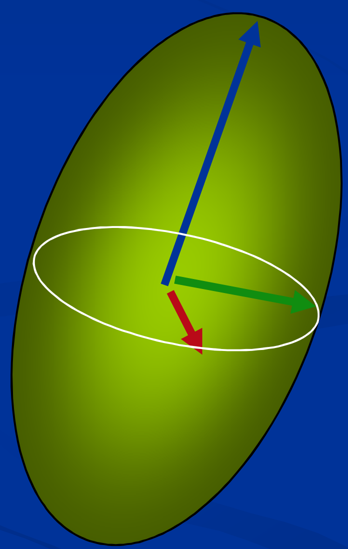
- Geometrically: EFG = tensor ellipsoid

  Asymmetry parameter:

  $\eta = (V_{xx} - V_{yy}) / V_{zz}$

- 2 main contrib. to the EFG at the nucleus:

1. the own e-shell (electronic contrib.)
2. the ligands (lattice contrib.)



Experimental determination of the EFG

Mößbauer spectroscopy

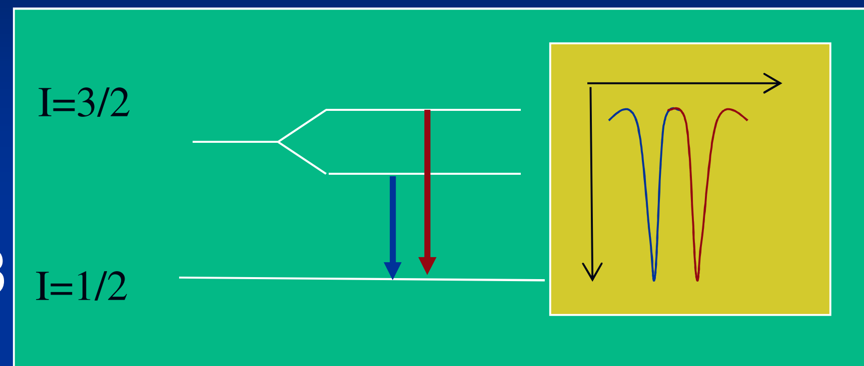
Quantity to be measured:

- Quadrupole splitting

  $QS = 1/2\ e\ Q\ V_{zz} \sqrt{1 + \eta^2/3}$

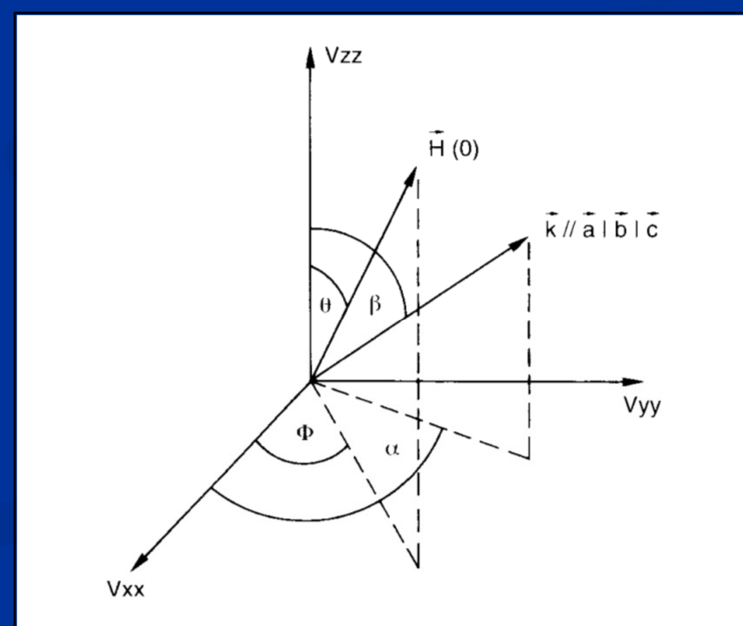
- Asymmetry parameter

  $\eta = (V_{xx} - V_{yy}) / V_{zz}$



With SCMBS additionally:

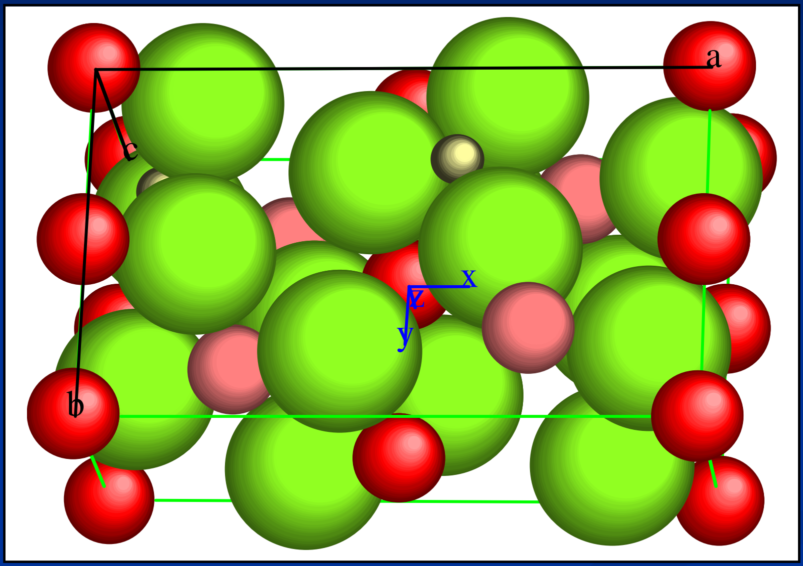
- Angle β betw. **k**-vector of the inc. γ-rays (=crystal axis) and V_{zz}
- Angle α betw. proj. of **k** to the (V_{xx}, V_{yy})-plane and V_{xx}



Semi-quantitative method/Nanoscope

- $\rho(x,y,z) = \sum_h \sum_k \sum_l A_{hkl}\, e^{-2\pi i\,(h^*x/a + k^*y/b + l^*z/c)}$
- A = Structure amplitude
- $|A_{hkl}| = 1/V_Z * |F_{hkl}|$
- $\rho(F_{obs}) - \rho(F_{cal,spherical}) =$
- $\Delta\rho_{aspherical}$ (Difference fourier)
- Idea: Aspherical densities-->EFG calc.
- Special software (Comp. tomography, DEDLOT under IDL®):
- EFG as wire frame graphics, calculated from difference electron densities (DEDs) on a Mac G5®

Example : synth. fayalite Fe_2SiO_4



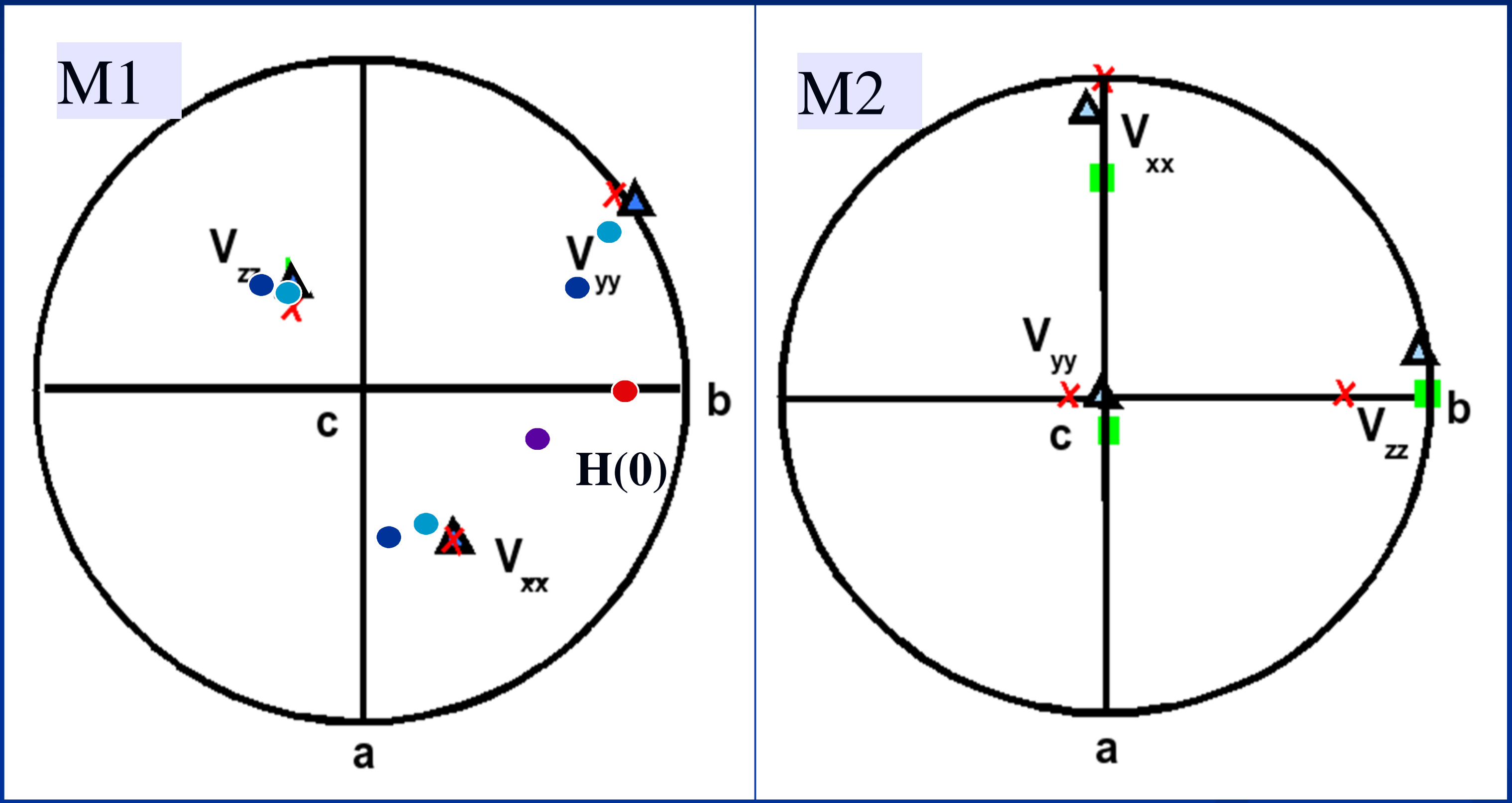
Synth. fayalite α-Fe_2SiO_4, orthorhombic, SG Pnma, Z=4

a = 1.0459(3), b = 0.6074(1), c = 0.4815(1) nm

Fe^{2+} -cations: M1(4a, PS -1) M2 (4c,PS m)

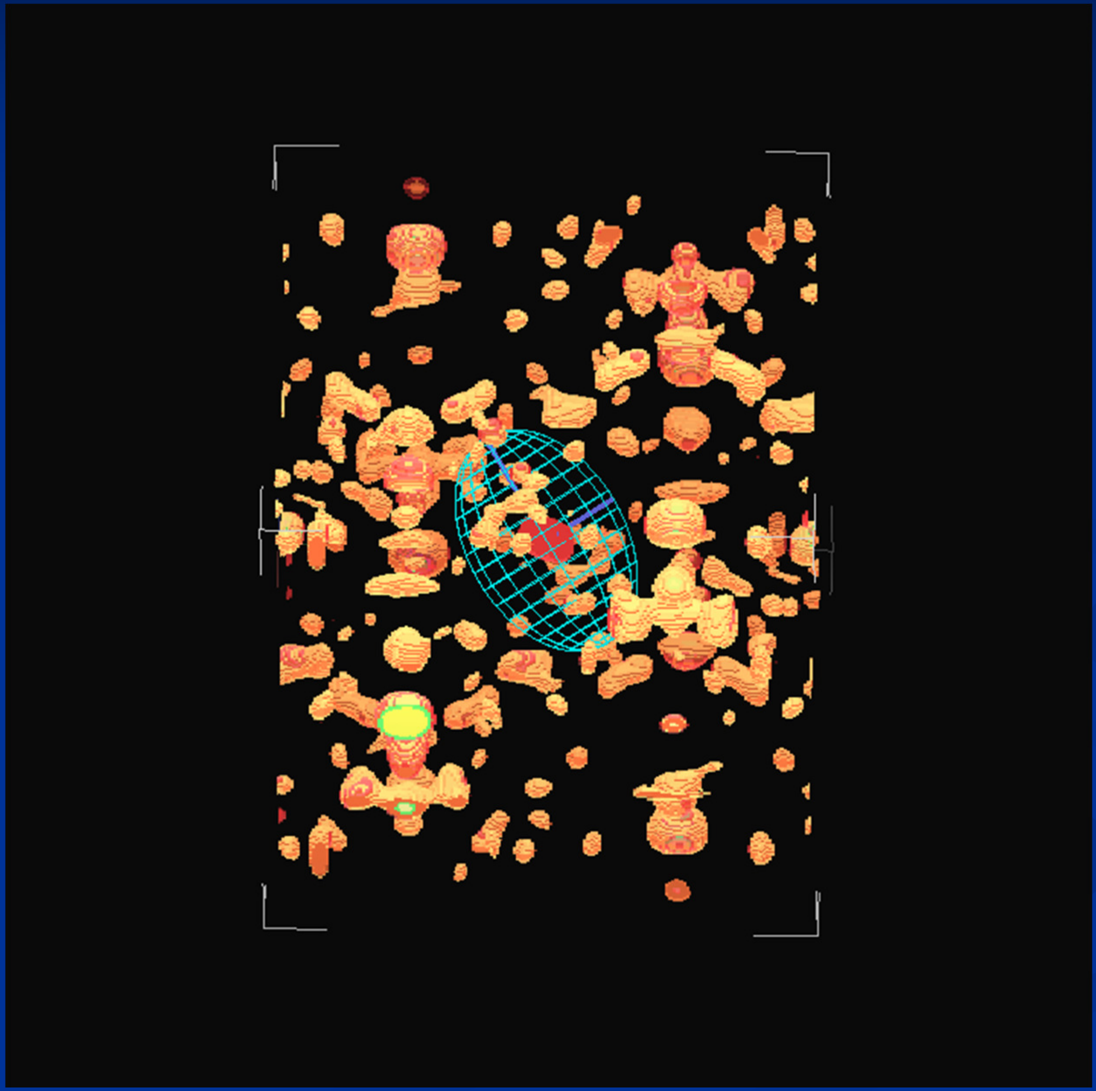
-->amazing structural u. magn. properties

Stereogram EFG + H(0)

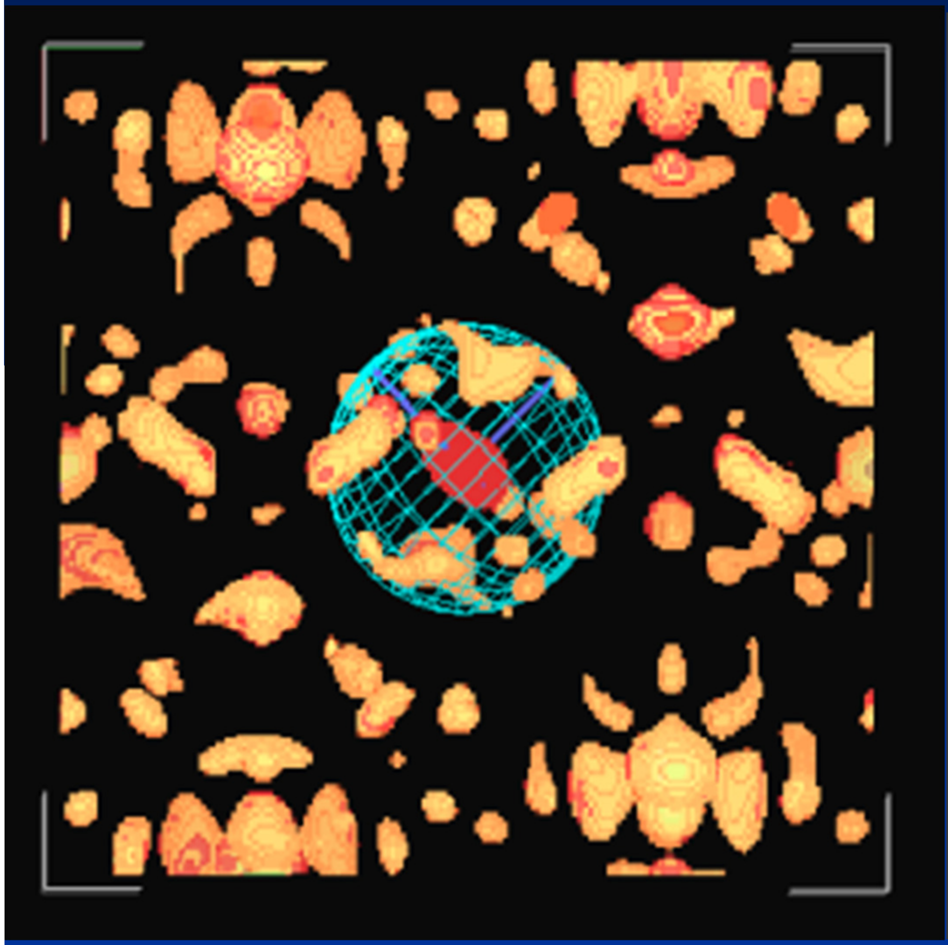


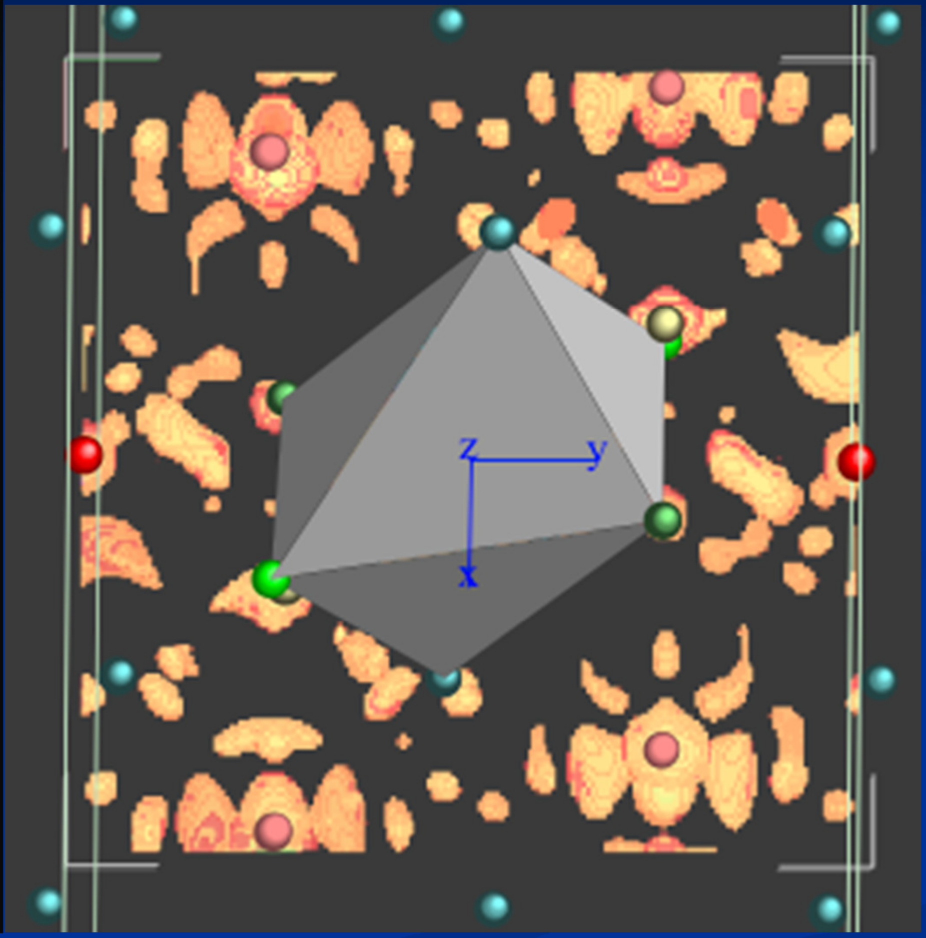
Lottermoser W, Forcher K, Amthauer G, Treutmann W, Hosoya S:
Phys Chem Miner 23 No. 7, 432 - 438 (1996)

DEN-Image

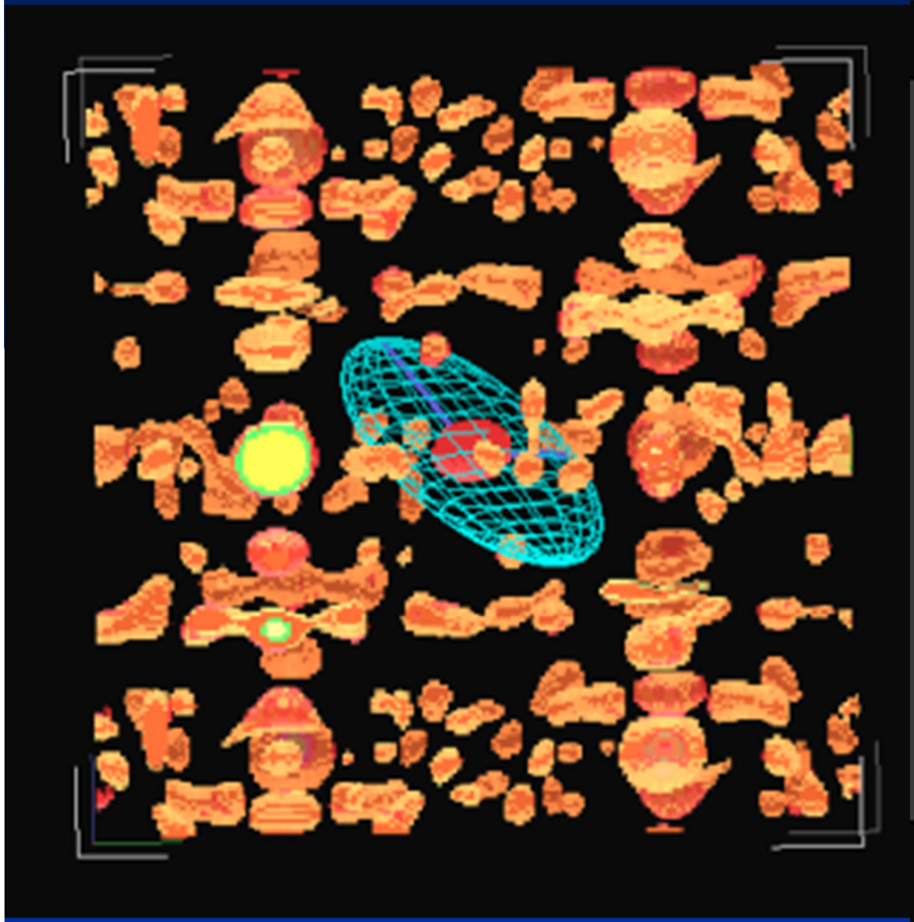


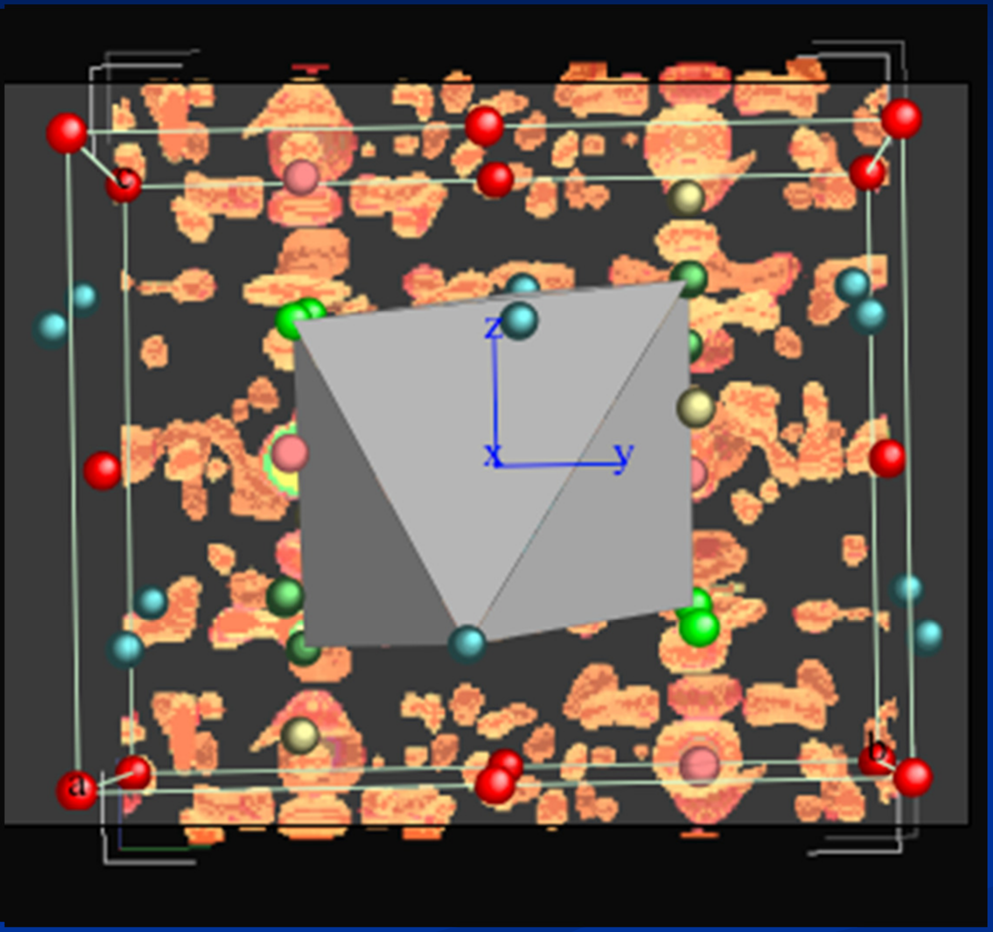
DEN images: M1 at 1/2 1/2 1/2: [001] DEDs + EFG | Oct.



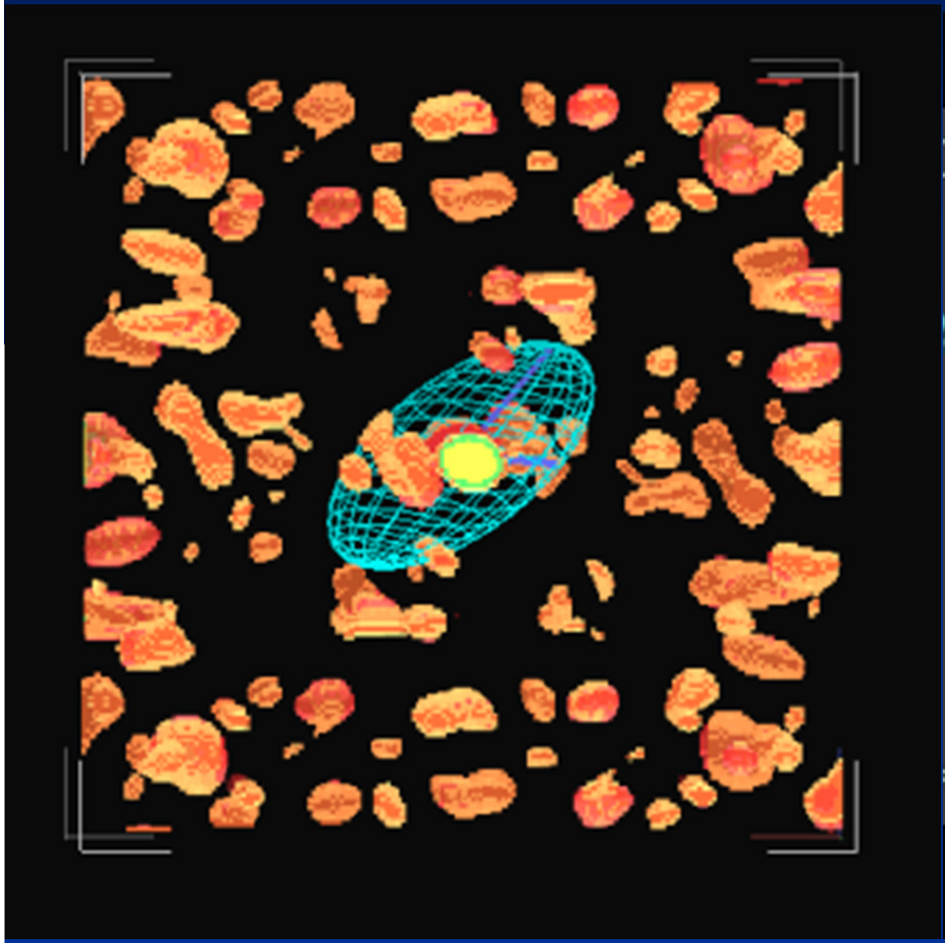


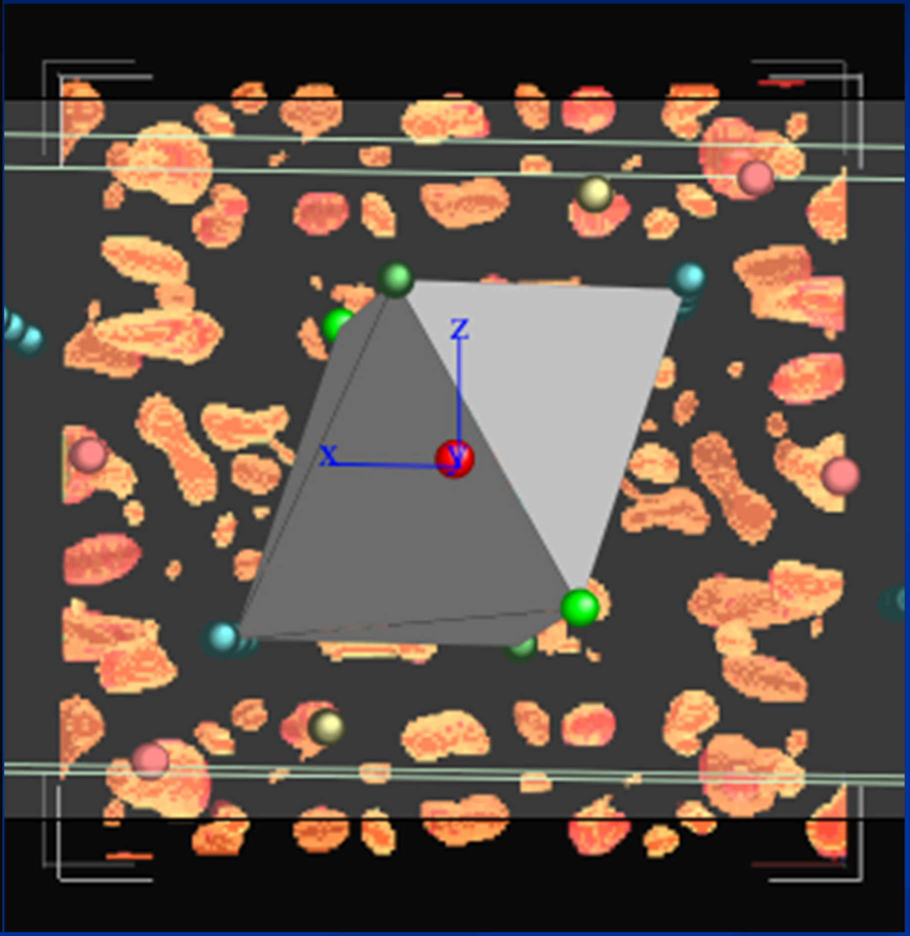
DEN images: M1 at 1/2 1/2 1/2: [100] DEDs + EFG | Oct.



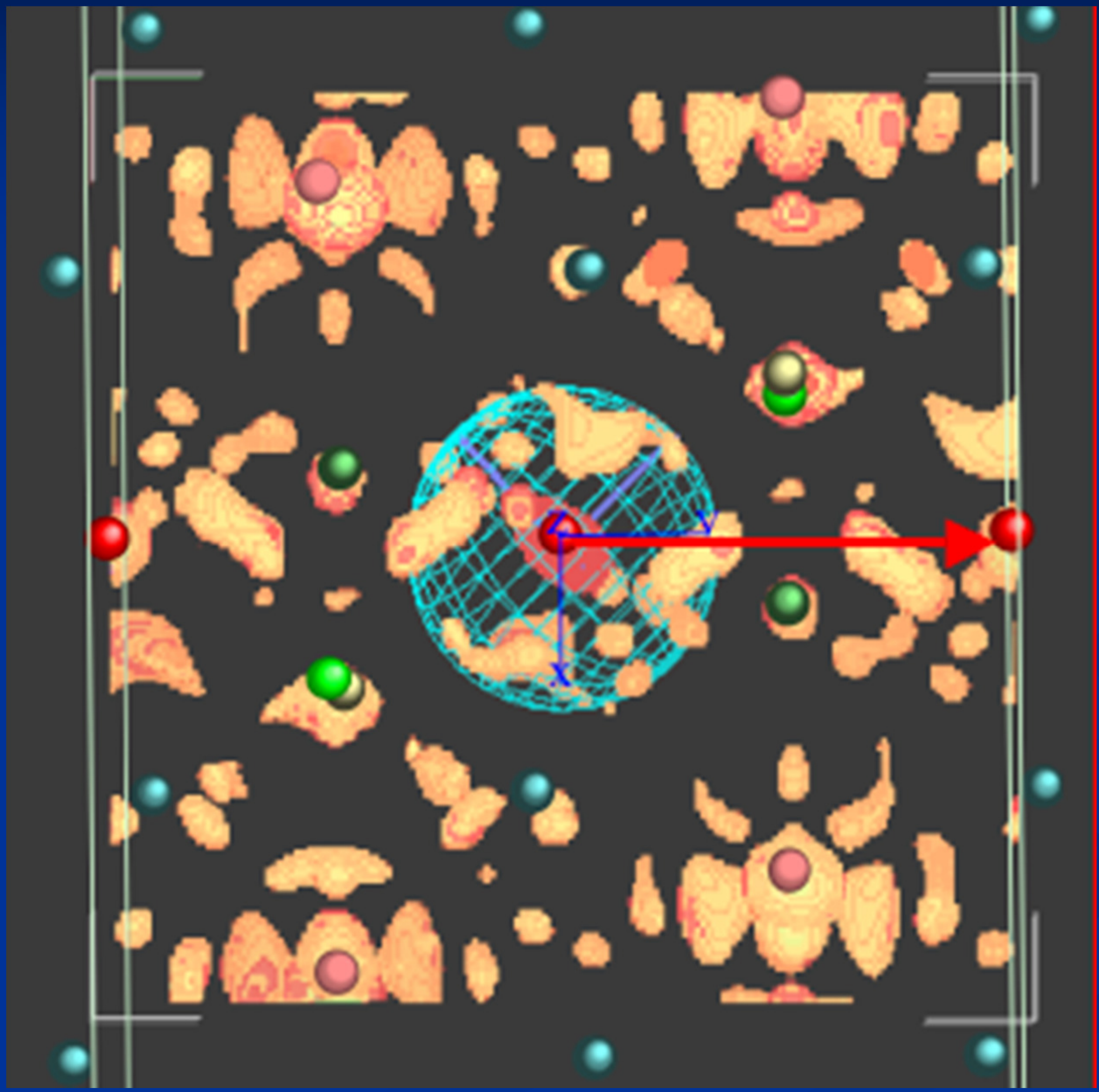


DEN images: M1 at 1/2 1/2 1/2: [010] DEDs + EFG | Oct.





DEN images: M1 at 1/2 1/2 1/2: [001] DEDs + H(0), T = 50K



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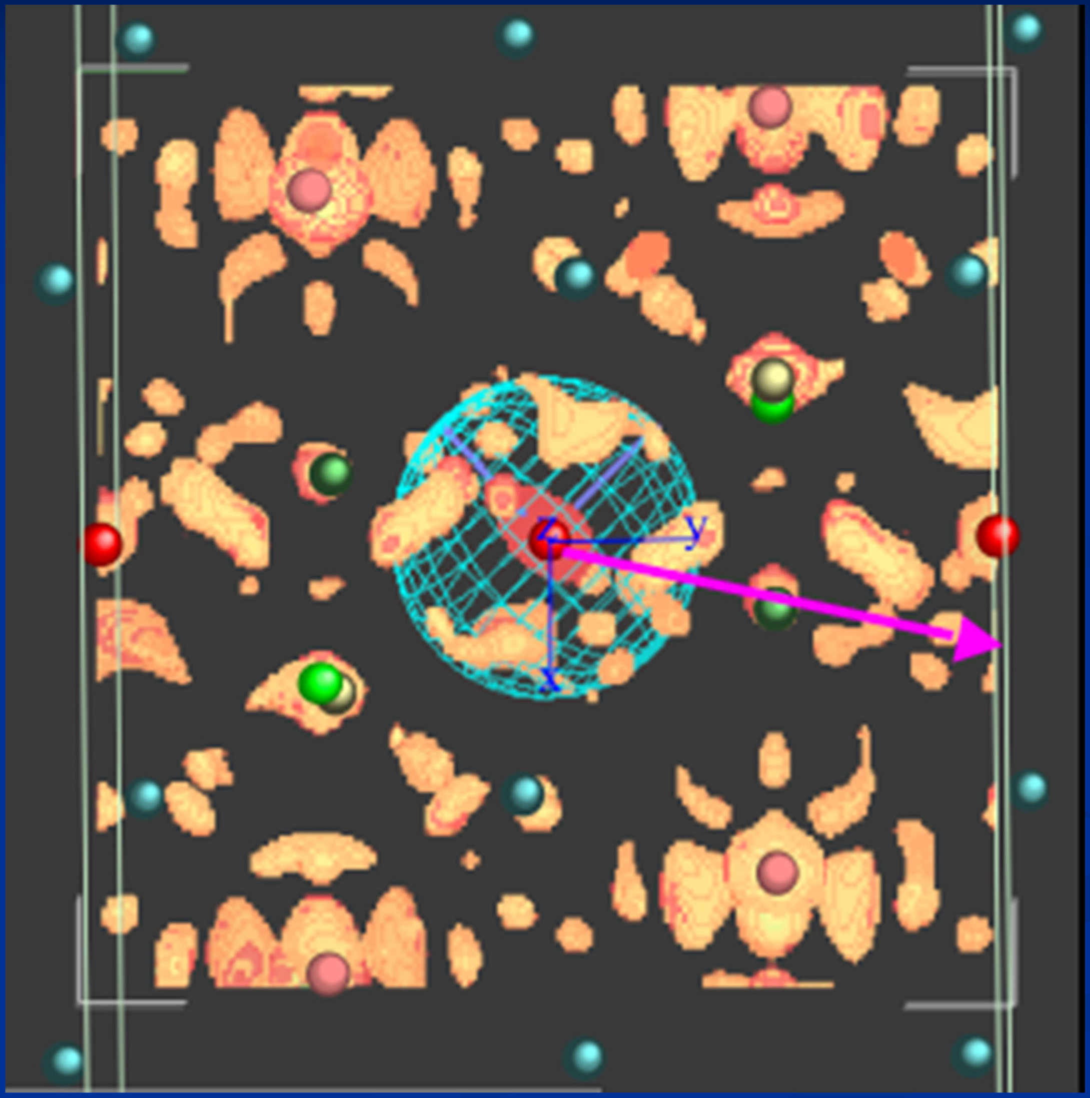
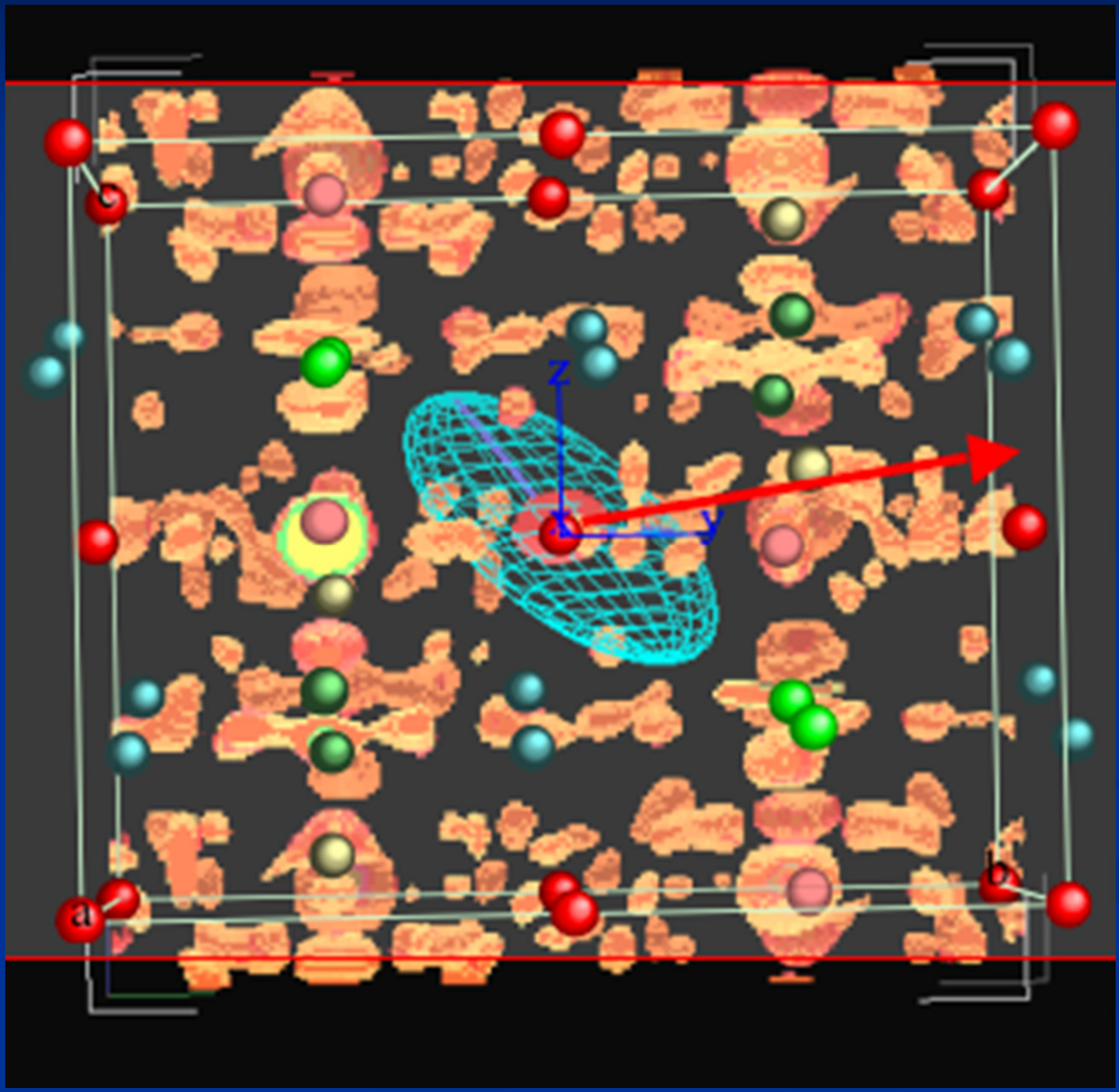
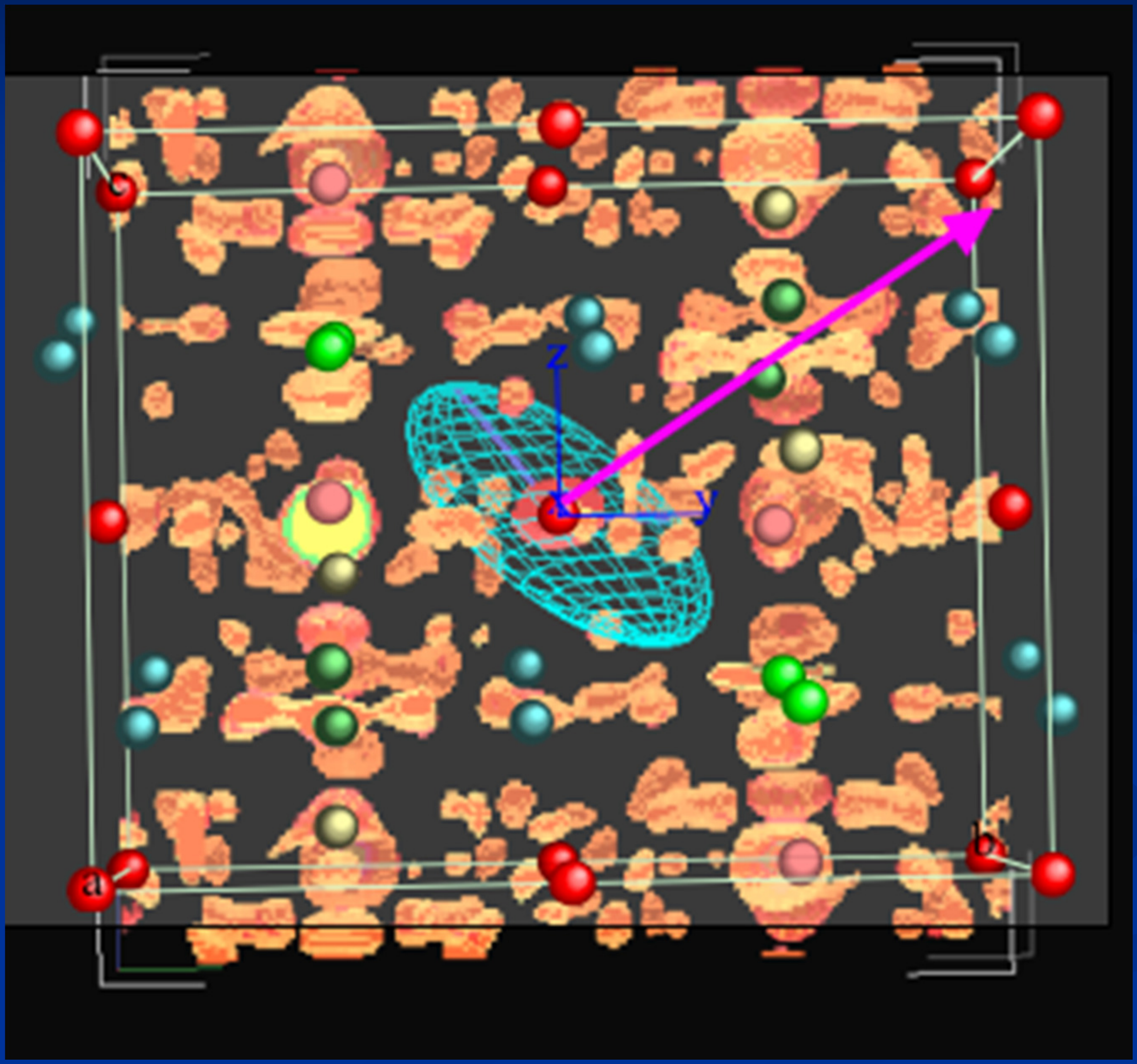


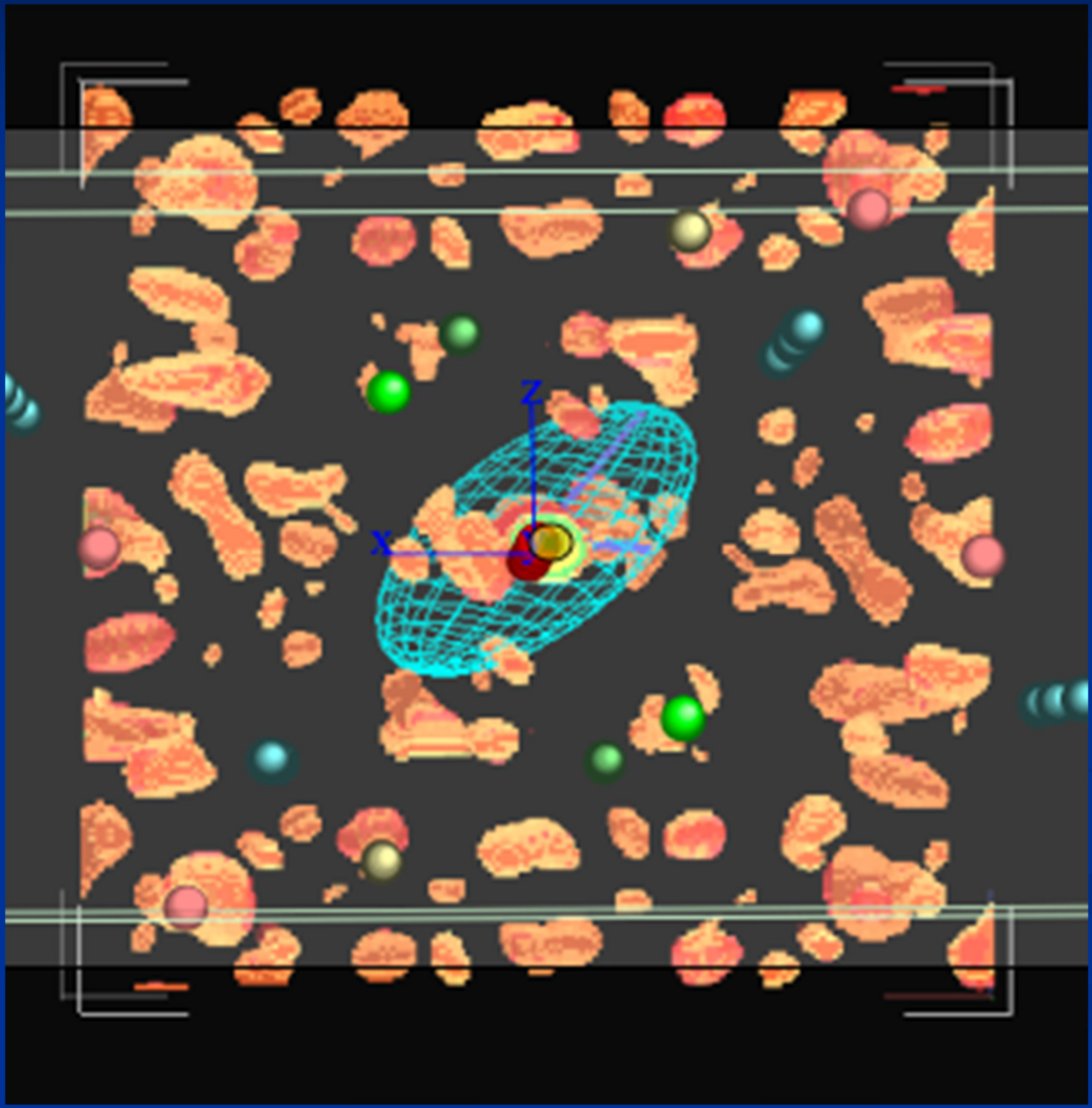
DEN images: M1 at 1/2 1/2 1/2: [100] DEDs + H(0), T = 50K



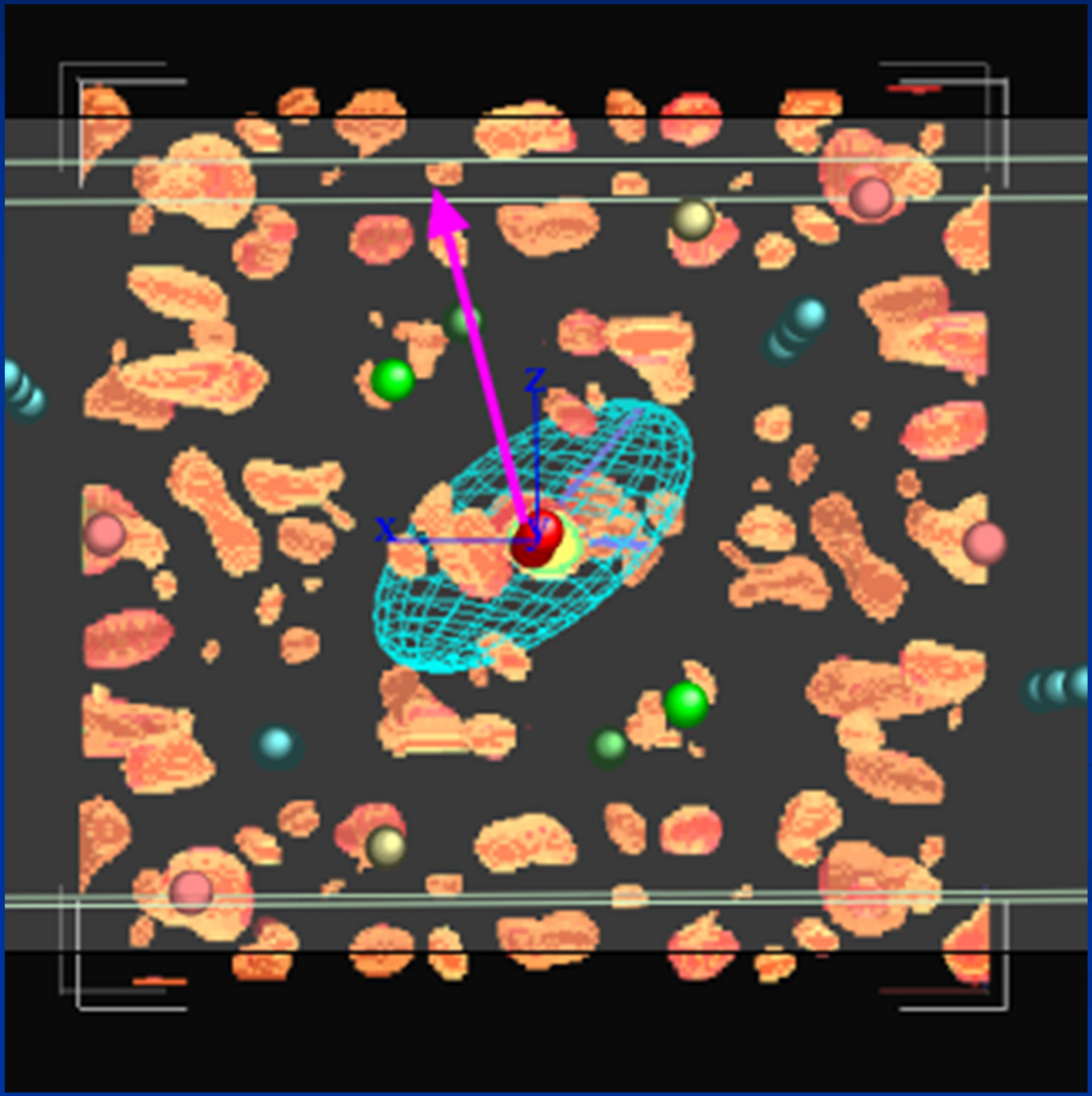
DEN images: M1 at 1/2 1/2 1/2: [100] DEDs + H(0), T = 10K



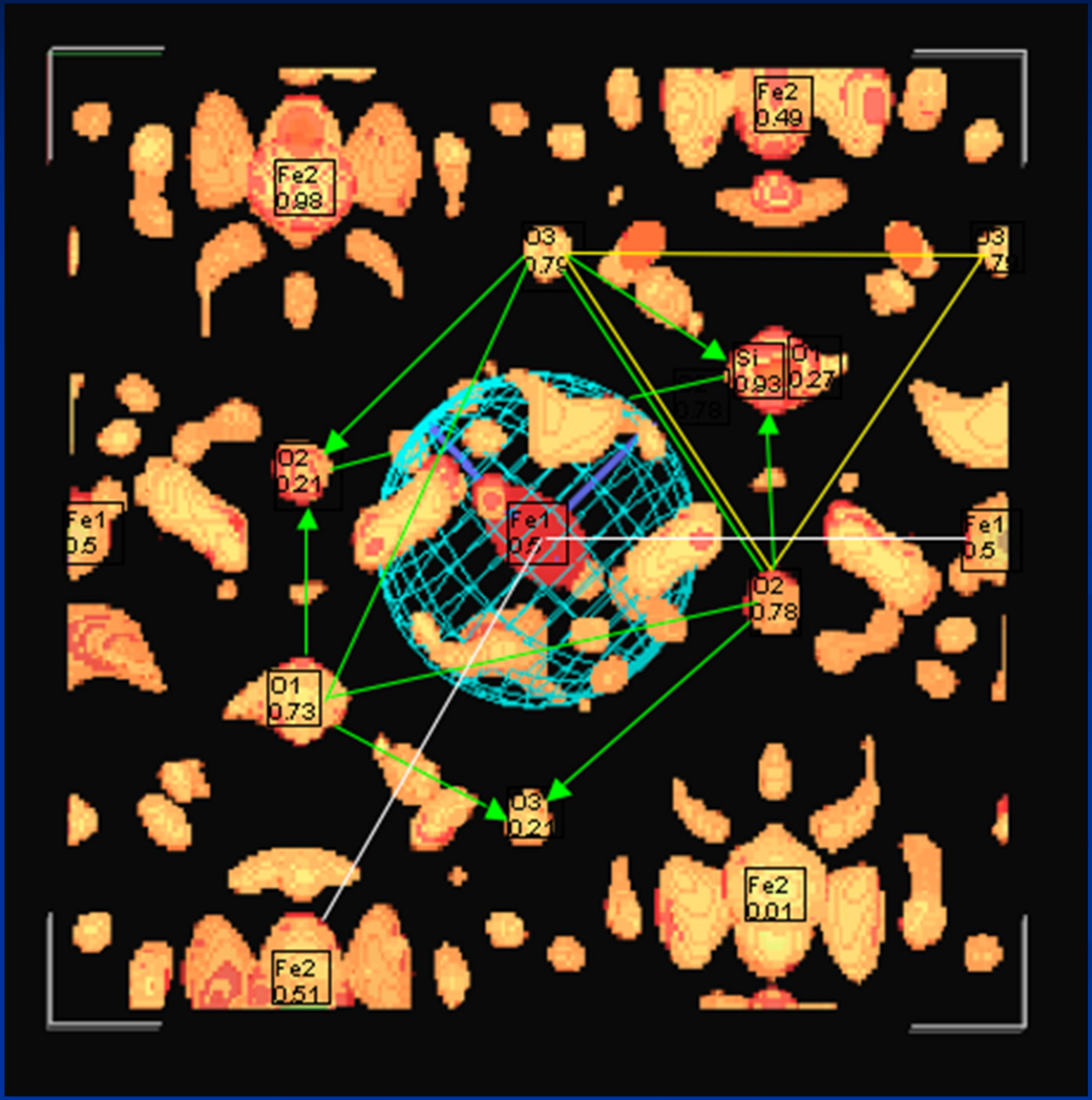
DEN images: M1 at 1/2 1/2 1/2: [010] DEDs + H(0), T = 50K



DEN images: M1 at 1/2 1/2 1/2: [010] DEDs + H(0), T = 10K



DEN images: M1 at 1/2 1/2 1/2: [001] DEDs + MO



Conclusions

- By application of the difference electron nanoscope (DEN) the electric field gradient (EFG) can be determined with high accuracy
- The EFG constitutes the link between (synchrotron-) diffractometry and spectroscopy (SCMBS or NQR/NMR)
- Essential for success is a multitude of exquisite structure factors preferably stemming from synchrotron diffraction measurements
- The difference electron densities (DEDs) within the unit cell may be viewed 3D with a wire frame model of the EFG

Conclusions

- It is possible to see amazing details like DED maxima around certain oxygens reponsible for superexchange coupling
- It should be possible to establish the DEN-method (semi-quant.) as another procedure to derive an EFG and direction of magnetic moments besides Mössbauer /NQR (exp.), neutron diffraction and DFT (full-quant.)

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