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The uniting of spectroscopy and diffractometry to the common benefit of nanoscience

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Several years ago, spectroscopy and diffractometry have still been treated as different methods with different kinds of scientific Conclusions. However, by our studies it has become possible to unify a special branch of spectroscopy, Single Crystal Mössbauer Spectroscopy (SCMBS)/NMR/NQR and, on the other hand, X-ray/Synchrotron and Neutron Diffractometry. Moreover, the results of DFT calculations could be implied as well. The common link is the electric field gradient that can be experimentally derived from the spectroscopic methods, theoretically by DFT and semi-quantitatively by diffractometry through Fourier inversion of difference electron densities (DEDs). We have created a special sophisticated software system which is able to show these DEDs floating three-dimensionally in space within the crystal unit cell together with the relevant efg. By this it is possible to gain an uncompared insight in structure-property relationships in as much as some of the above spectroscopic and diffractometric methods are sensitive to magnetism. For the first time, at least to our knowledge, real (not simulated!) atomic/molecular 3d orbitals can be seen by the viewer, the reason due to which the method is called Difference Electron Nanoscope (DEN). Since 3D viewing on a screen without tools is difficult to achieve, a special procedure is applied to perform a rather striking 3D imaging. The method is demonstrated on special examples. With further achievements in synchrotron diffraction and data processing, however, it should be possible to dispose of an online-version of the DEN within a couple of years.

Biography

Werner Lottermoser has completed his thesis work about neutron diffraction and magnetism of special silicates from Francfort University (Germany) and University Lecturing Qualification on Single Crystal Mössbauer Spectroscopy (SCMBS) in 1996 from Salzburg University (Austria). He is now working on sub-nanometric imaging, nanomaterials and materials for industrial applications. He has published more than 65 papers in reputed journals and 150 abstracts and has been serving e.g. for one year as a referee board member at the *Journal of Physical Chemistry* A. Recently, he was awarded the Austrian Staatspreis for Innovation together with AB-Microelectronics, Salzburg.

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