# A Spherical Harmonic Oscillator Basis for Reduced Bandwidth Requirements

Paul F Baumeister Jülich Supercomputing Centre, Forschungszentrum Jülich, Germany

JÜLICH Forschungszentrum

Large scale electronic structure calculations require modern HPC resources and, as important, mature HPC applications that can make efficient use of those. Real-space grid-based applications of Density Functional Theory using the Projector Augmented Wave method can give the same accuracy as DFT codes relying on a plane wave basis set but exhibit an improved scalability on distributed memory machines. The projection operations of the PAW Hamiltonian are known to be the most performance critical part due to their limitation by the available memory bandwidth. We investigate on the usability of a 3D factorizable basis of Hermite functions for the atomic PAW projector functions that allows to reduce and nearly to remove the bandwidth requirements for the grid representation of the projector functions in projection operations. This increases the fraction of exploitable floating-point operations on modern vectorized many-core architectures, like GPUs, by raising the arithmetic intensity of such operations.

## 1D Harmonic Oscillator

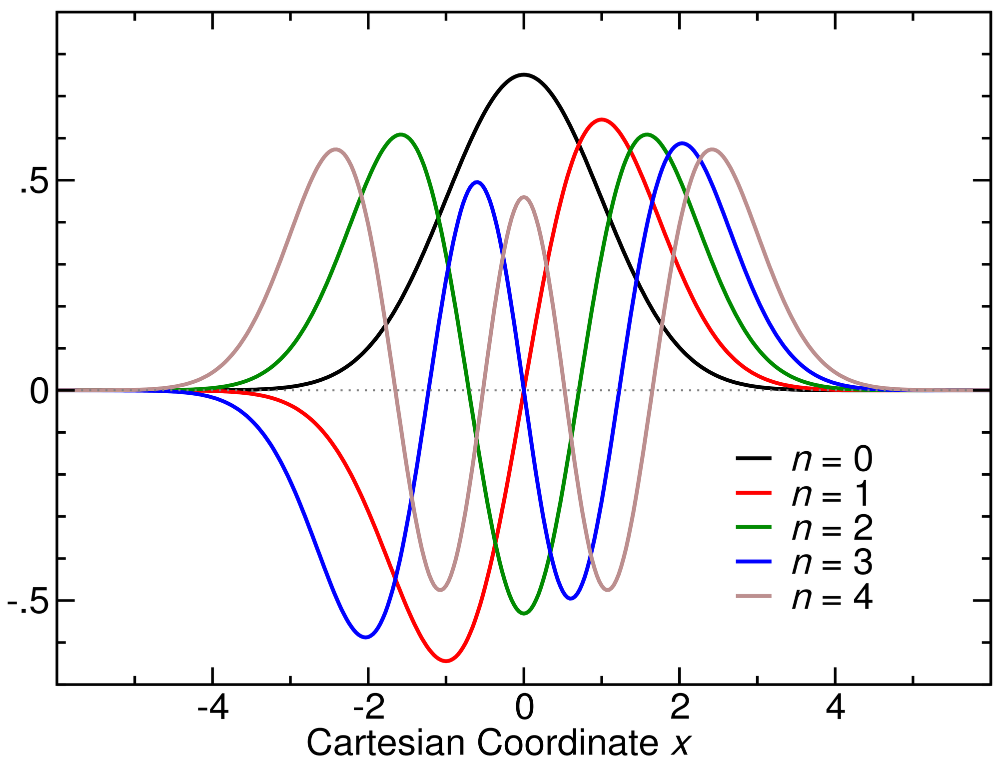
$$\hat{H}_{\text{HO}} = \hat{T}_{\text{kinetic}} + \hat{V}_{\text{potential}} = -\frac{\partial^2}{\partial x^2} + x^2$$

$$\psi_{\text{HO}}(x) \sim H_n(x) \cdot \exp(-x^2/2)$$

### Hermite polynomial · Gaussian


Ch. Hermite


J. C. F. Gauss




Recursive definition of Hermite polynomials

$$H_{n+1}(x) = xH_n(x) - \frac{n}{2}H_{n-1}(x)$$

$$H_0(x) = 1,\ H_1(x) = x,\ H_2(x) = x^2 - \frac{1}{2}$$

## Application to Electronic Structure Calculations on Cartesian Grids

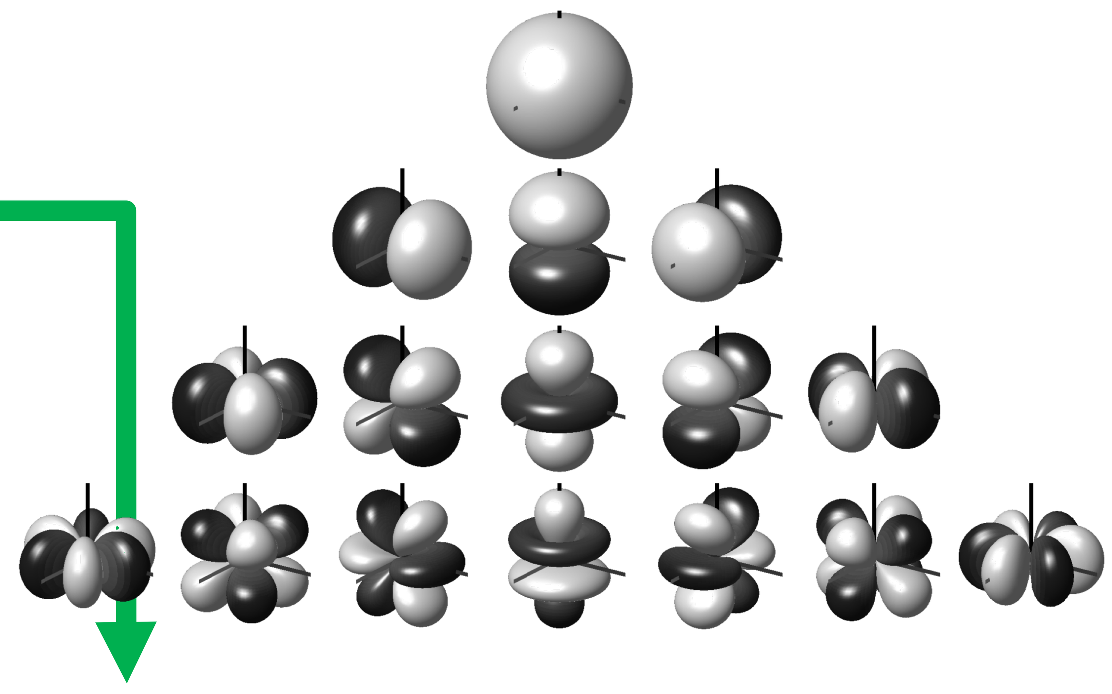
For reasons of parallel scalability, the quantum mechanical wave functions in Density Functional Theory (DFT) are represented on 3D Cartesian grids. Using the Projector Augmented Wave (PAW) method [Blöchl95], a non-local operator accurately describes the scattering of valence electrons at the ions.

$$\hat{V}_{\text{ion}} = |\tilde{p}_i\rangle\, D_{ij}\, \langle\tilde{p}_j|$$

The non-locality can be implemented as projection and expansion operations with a set of localized functions refered to as projectors. If we manage to represent the projectors in a small SHO basis, we can omit storing and loading of precomputed projector function values in both, projection and expansion operation. This releases memory capacity constraints and, even more important, reduces the requirements for memory bandwidth which has become the most costly resource in HPC.
The 1D HO basis functions are cheap enough to be generated on-the-fly.

## 3D Spherical Harmonic Oscillator

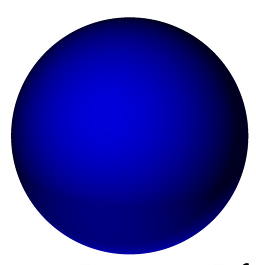
$$\hat{H}_{\text{SHO}} = -\vec{\nabla}^2 + \vec{r}^2$$
$$= -\Delta + r^2$$
$$= \hat{H}^{[x]}_{\text{HO}} + \hat{H}^{[y]}_{\text{HO}} + \hat{H}^{[z]}_{\text{HO}}$$

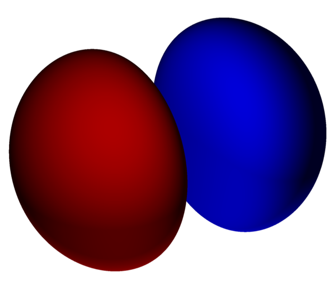


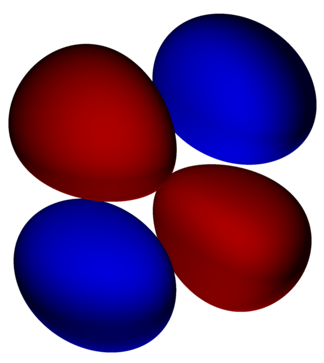
### Cartesian Representation

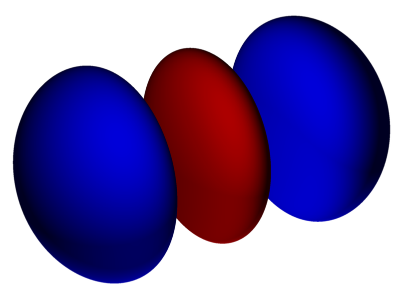
$$\Psi_{\text{SHO}}(x,y,z) = \psi_{n_x}(x)\psi_{n_y}(y)\psi_{n_z}(z)$$

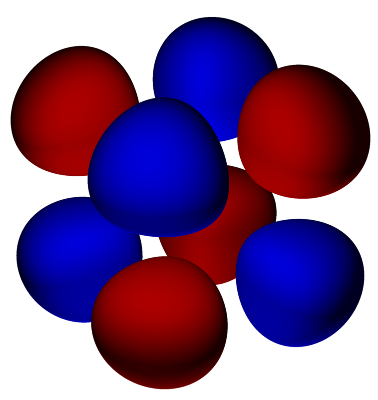
as 3D Cartesian product of 1D-HO eigenfunctions
→ Tensor compression

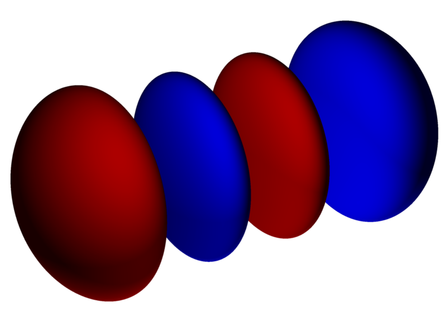

*s* [000][1]

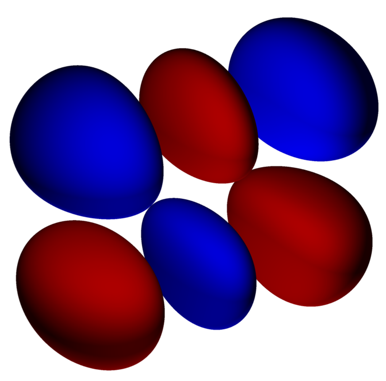

*p* [100][3]


*d* [110][3]


[200][3]


*f* [111][1]


[300][3]


[210][6]

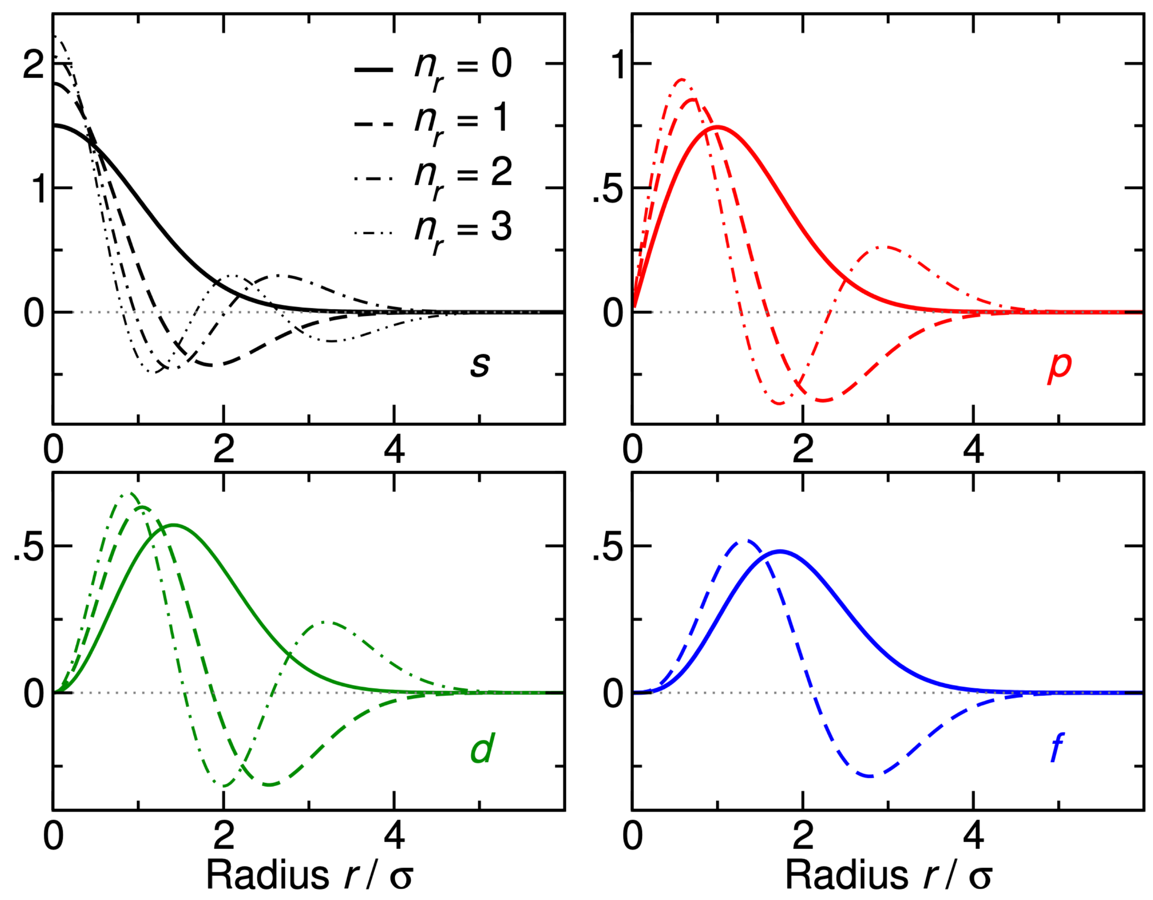
### Radial Representation

$$\Psi_{\text{SHO}}(r,\vartheta,\varphi) = R_{n_r\ell}(r) \cdot Y_{\ell m}(\vartheta,\varphi)$$


E. Laguerre

Spherical Harmonics

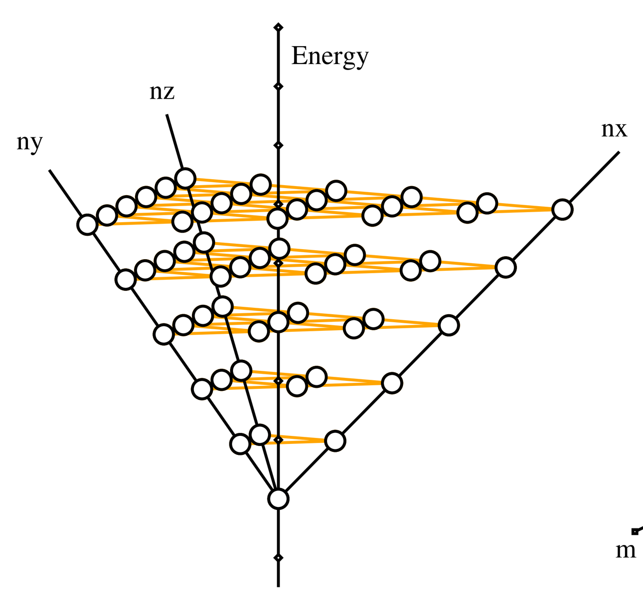
$$R_{n_r\ell}(r) \sim r^\ell L^{(\ell+\frac{1}{2})}_{n_r}(r^2)\exp(-r^2/2)$$



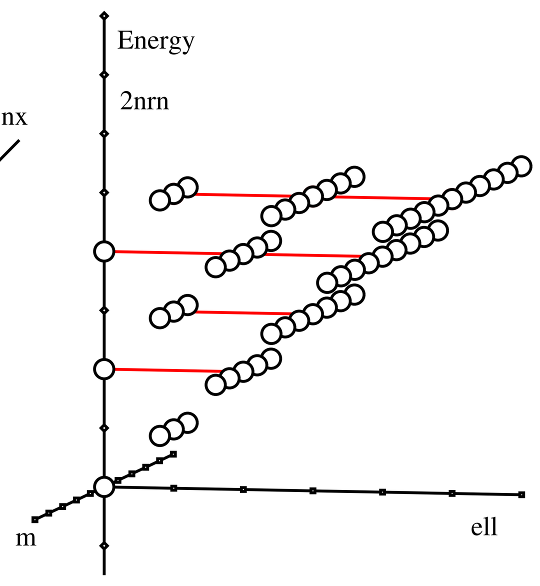

Paper@arXiv 1905.00480

## Energy Degeneracy

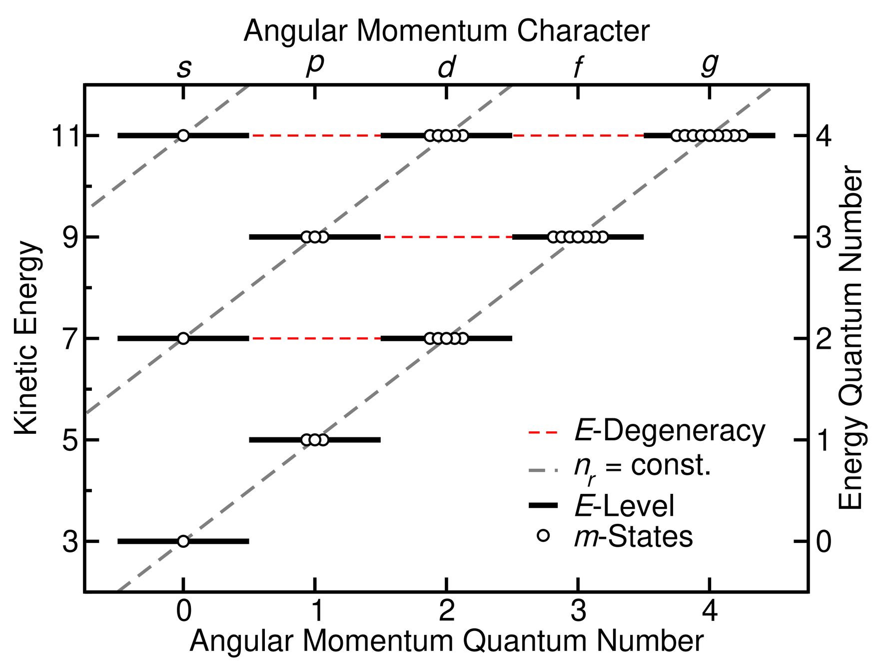
$$E = 2(n_x + n_y + n_z) + 3 \qquad E = 2(\ell + 2n_r) + 3$$



Cartesian



Radial




## Unitary Transformation in energy-degenerate subspaces

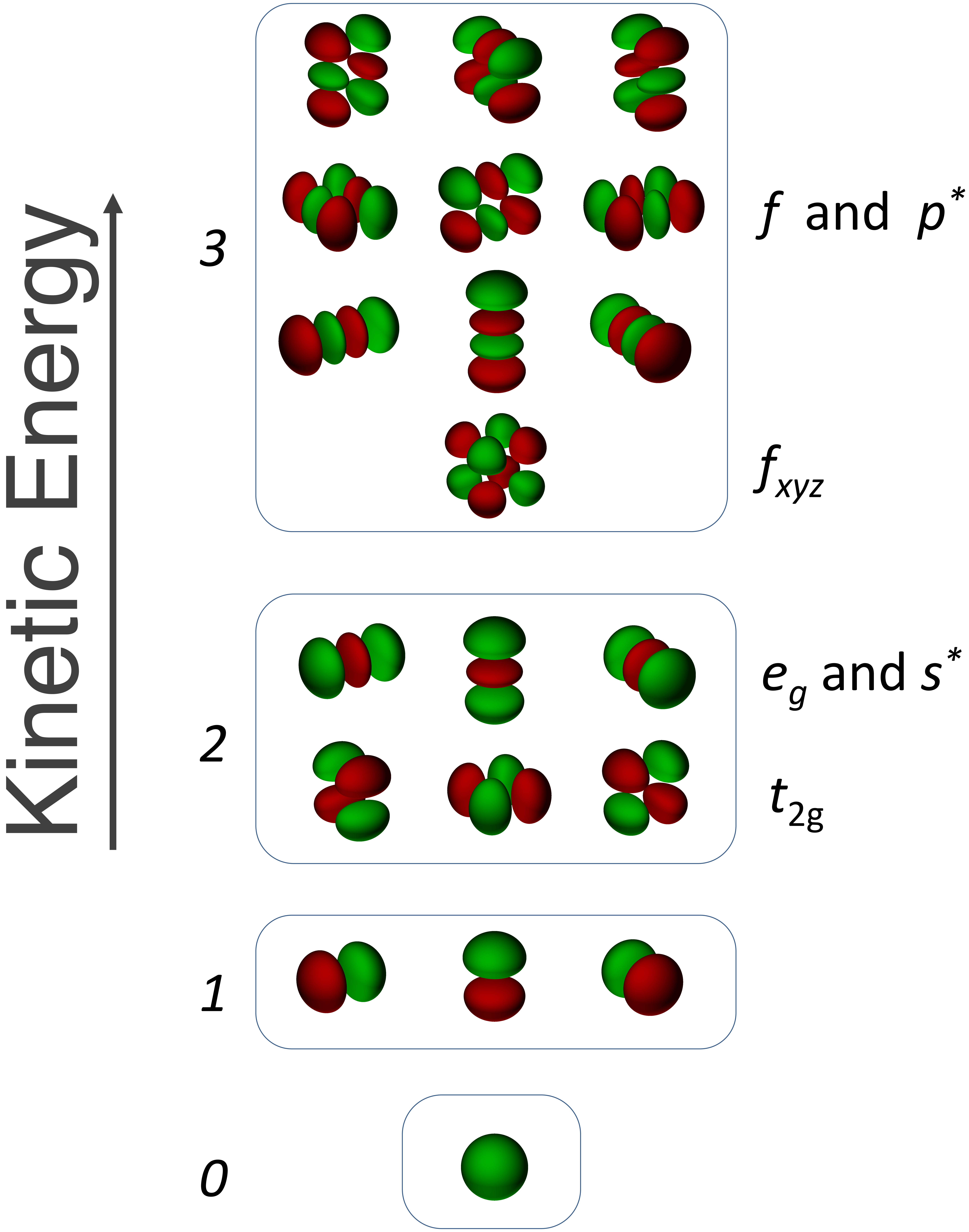
$$\Psi_{n_x n_y n_z}(x,y,z) \equiv \sum_{n_r \ell m} U^{n_r \ell m}_{n_x n_y n_z}\ \Psi_{n_r \ell m}(r,\vartheta,\varphi)$$

Angular momentum characters

$$s^* \oplus d,\quad p^* \oplus f,\quad s^{**} \oplus d^* \oplus g,\ \ldots$$

# A Spherical Harmonic Oscillator Basis for Reduced Bandwidth Requirements

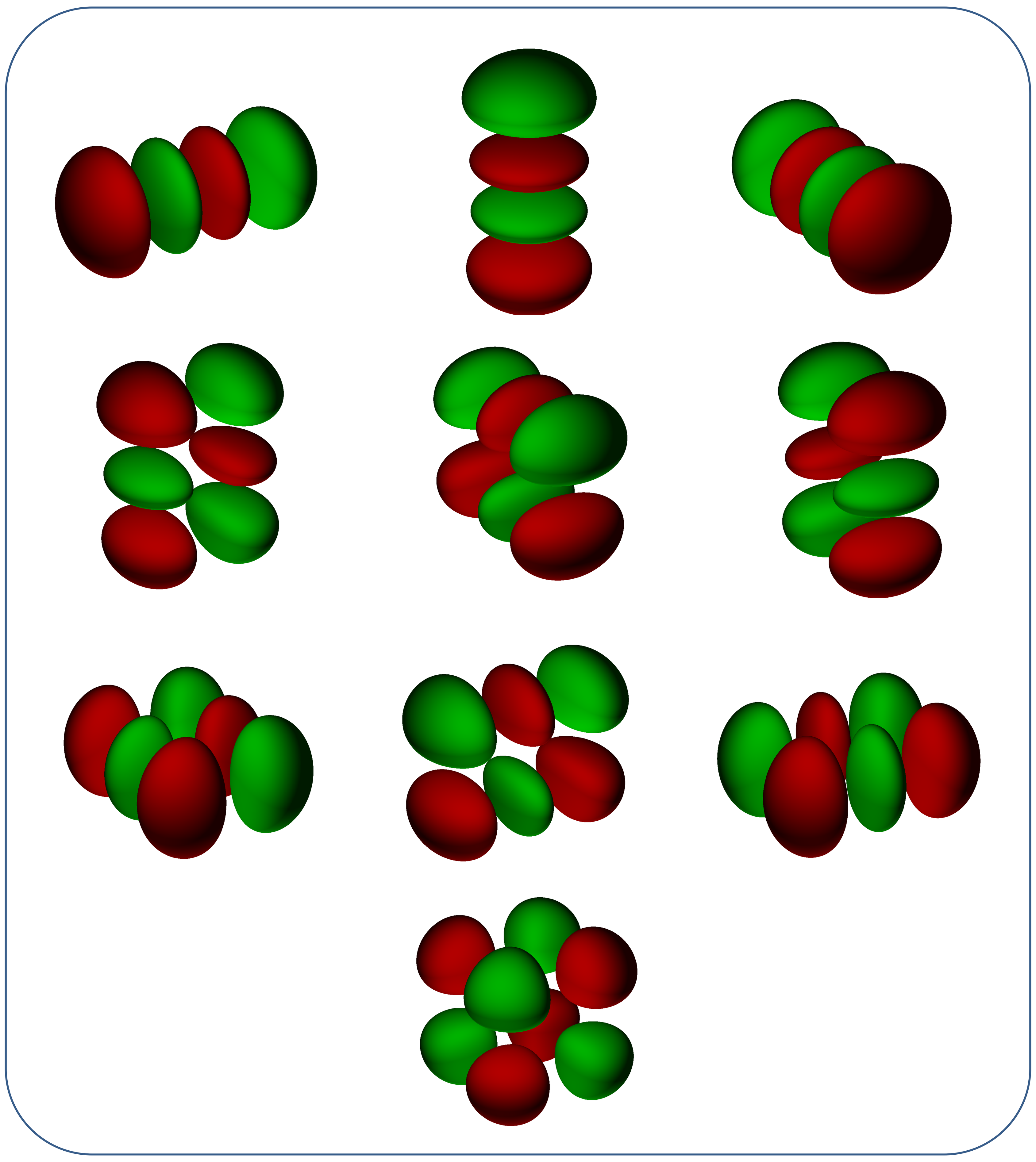
Paul F Baumeister (JSC, Germany)

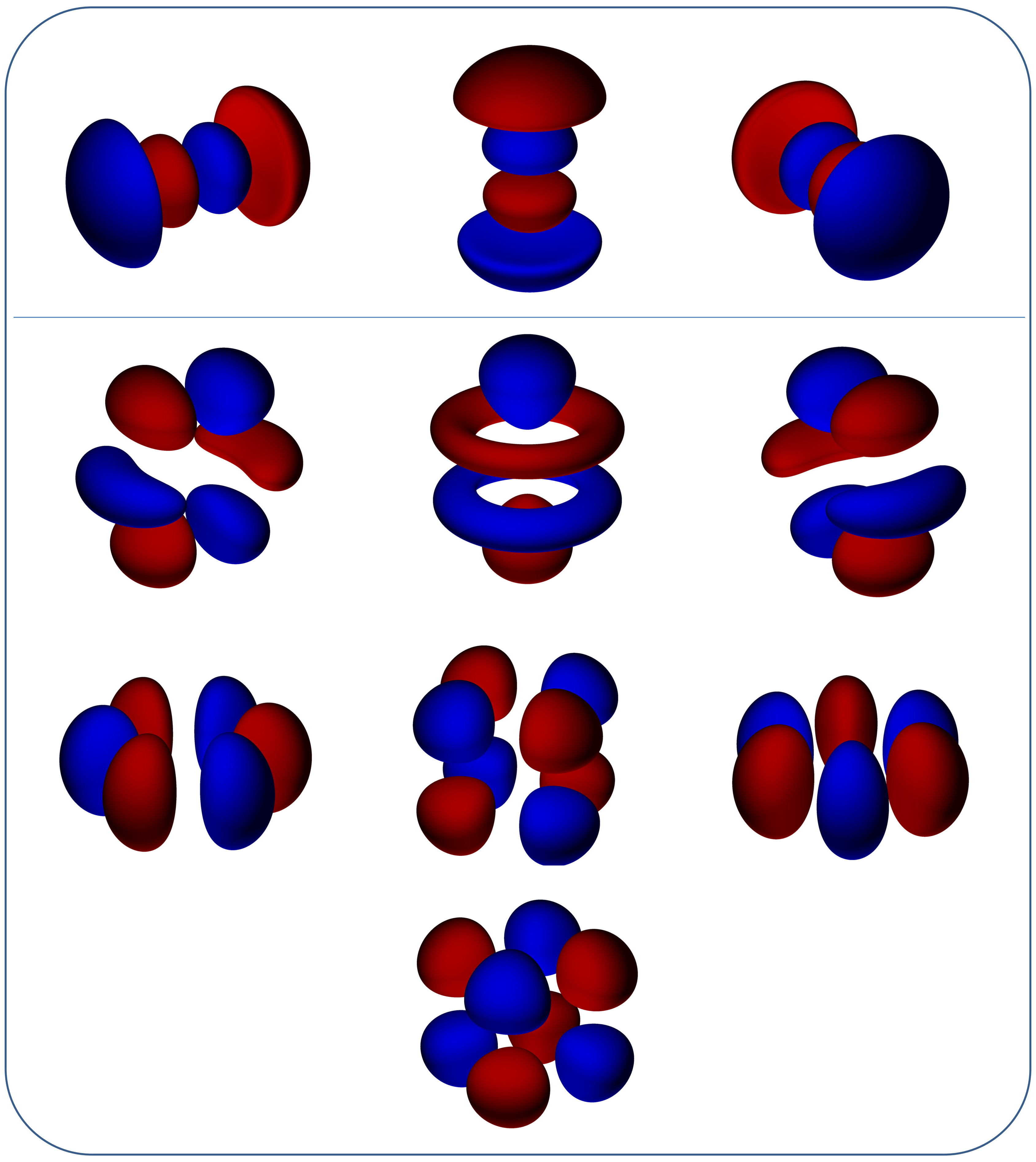


# A Spherical Harmonic Oscillator Basis for Reduced Bandwidth Requirements

Paul F Baumeister (JSC, Germany)

JÜLICH Forschungszentrum





Cartesian factorizable

Spherical harmonics