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Title:	Actinides: What we should do and what we do--and how to connect the two
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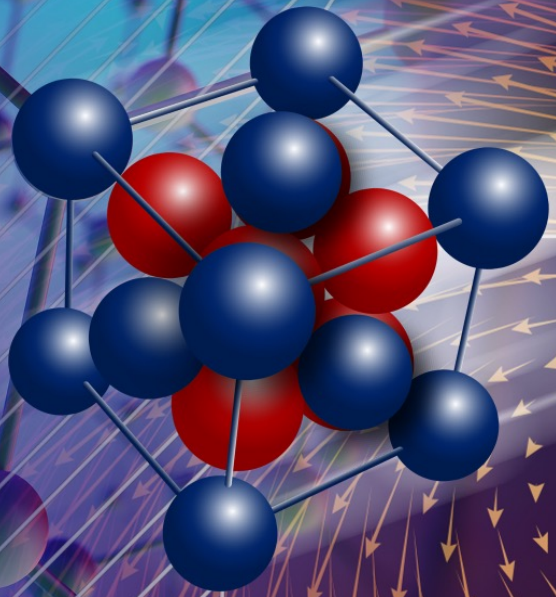
Los Alamos NATIONAL LABORATORY

Los Alamos Materials

Actinides: What we should do and what we do—and how to connect the two

Ann E. Mattsson Wills,
Materials and Physics data, XCP-5

May 9, 2023



NNSA National Nuclear Security Administration
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Real world of actinides (relativistic materials), Experiments

What we should do

Dirac equation

orbitals to densitals

Dirac-based DFT

Orbital: Ψ_i not an observable

Electron density: $\Sigma_i f_i |\Psi_i|^2$ an observable

Probability density: $|\Psi_i|^2$

Densital: $|\Psi_i|^2 >$ cutoff

Schrödinger equation

orbitals to densitals

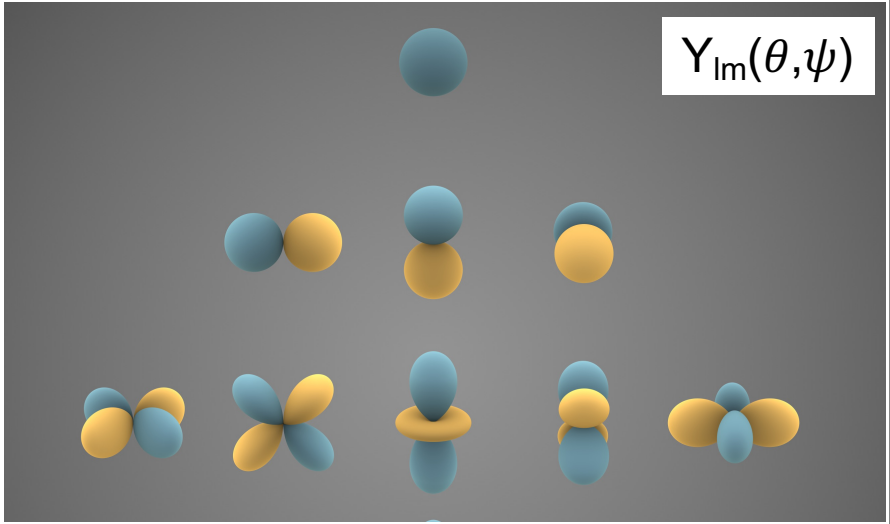
SE-based DFT

Non-relativistic limit

What we do

Orbitals

n,l,m,spin



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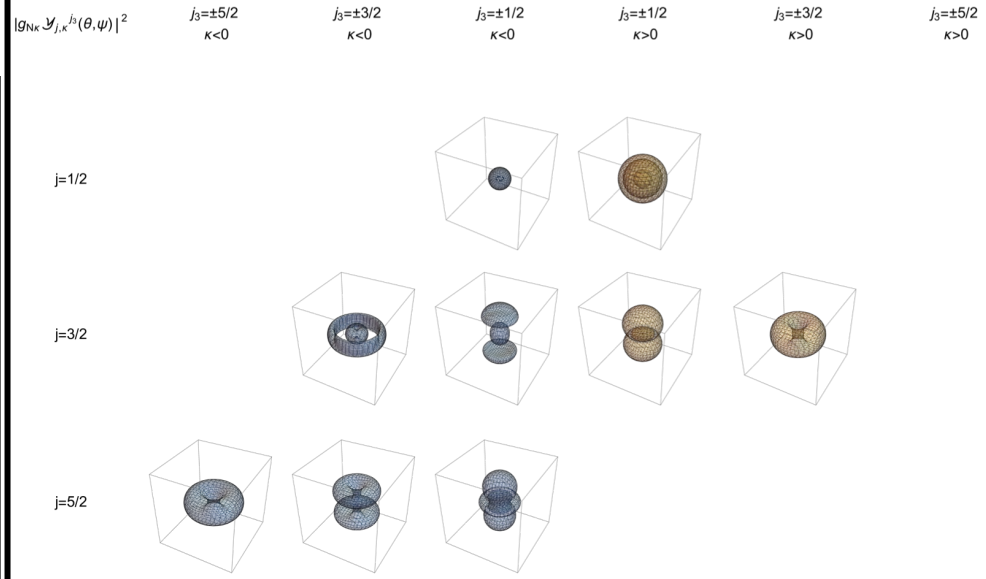
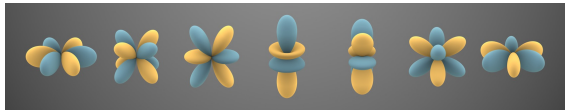
Densitals

N, j, j_3, κ



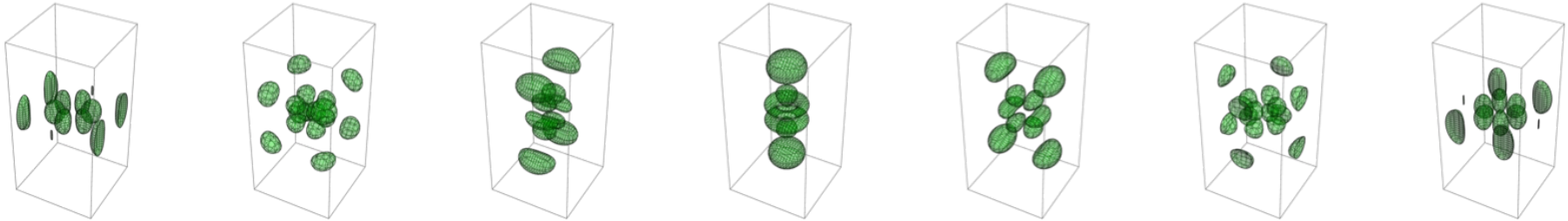
Hydrogen-like atom with non-interacting electrons



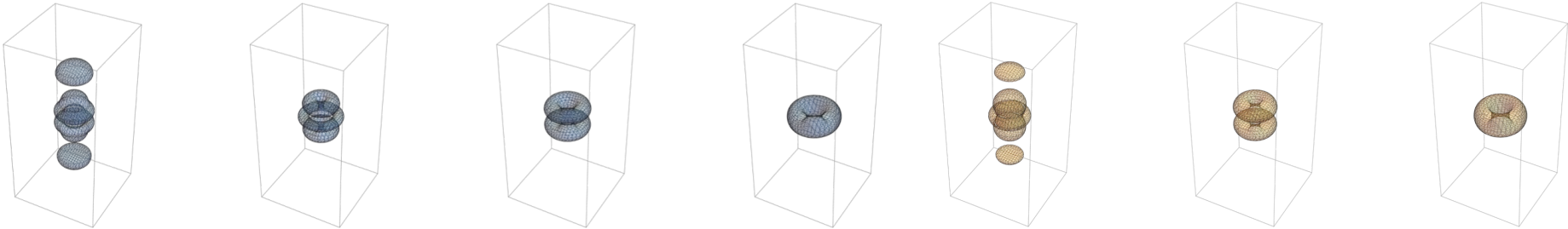
Schrödinger Equation

Real spherical harmonics

5f m=-3,-2,-1,0,1,2,3
Spin-up and spin-down
gives 14 electrons



Dirac Equation

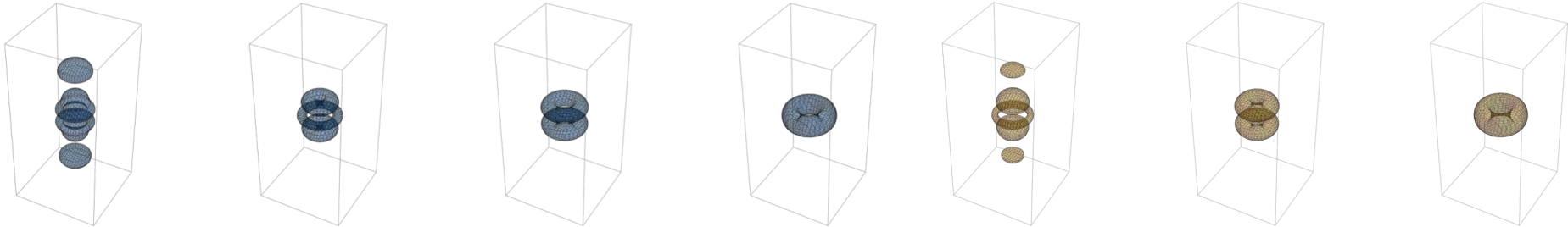


$5D^{h}f$ (4 each of $\pm j_3$), $5D^{l}f$ (3 each of $\pm j_3$) total 14 electrons

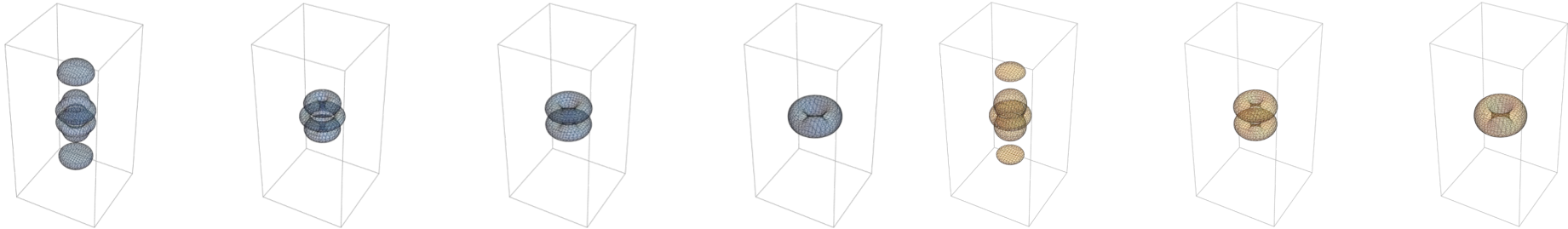
Hydrogen-like atom with non-interacting electrons

Dirac spherical harmonics

Schrödinger Equation



Dirac Equation



$5D^{h}f$ (4 each of $\pm j_3$), $5D^{l}f$ (3 each of $\pm j_3$) total 14 electrons

As no Dirac-DFT codes are available (yet) we need to interpret Schrödinger equation solutions from a Dirac equation viewpoint.

We can get densitals from the Schrödinger equation that correspond well to the Dirac densitals for the same problem.

Future work: Use the insights gained from this new viewpoint to revolutionize DFT based calculations for actinides.

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