A Heuristics-Based Approach to the Prediction of FODs in Fermi-Lowdin Orbital Self Interaction Correction (FLOSIC) Theory

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The FLOSIC Method

The Fermi-Lowdin Orbital (FLOs)

The Fermi-Lowdin Orbital Descriptors (FODs)

The NRLMOL Code

- Describe the code and status of usability

Overview of Code

- Big-picture description of how the code works.

FOD Determination and Practical Considerations

- Describe methods used to input FODs into the FLOSIC program.

- Prime motivation behind this project: an automated and faster process to begin calculations, informed from "empirical" data, capable to extending to larger systems.

FOD Geometric Motifs

- Describe how FODs arrange themselves similar to LDQ Theory. This (emergent?) behavior makes it

SP3 Arrangements

SP3D Arrangement

Dominance Schema

- Sometimes FODs are closer to atoms that are of lesser atomic number Z than the neighbouring heavier atoms. This could be attributed to shielding caused by the filled shells of periods 3 and above. The behavior is described in Figure 1. This will play a special part in the prediction of bonding FODs.

$n = m = 2$	$n = 2, m > n$	$n = m > 2$	$n \neq m, n \neq 2, m \neq 2$
No shielding electrons. Tighter BFOD.	Shielding electrons of m repel BFOD. Biased towards lighter atom	The BFOD are repelled away from the bonding axis	Favor the lower period

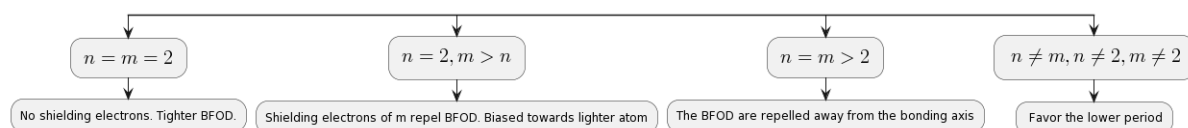Figure 1: dominance

The FOD-Lego Program

- Note: Different name needed probably

General Overview

- Give a **Big-Picture** overview as seen in image Figure 2

General Overview of FODLego
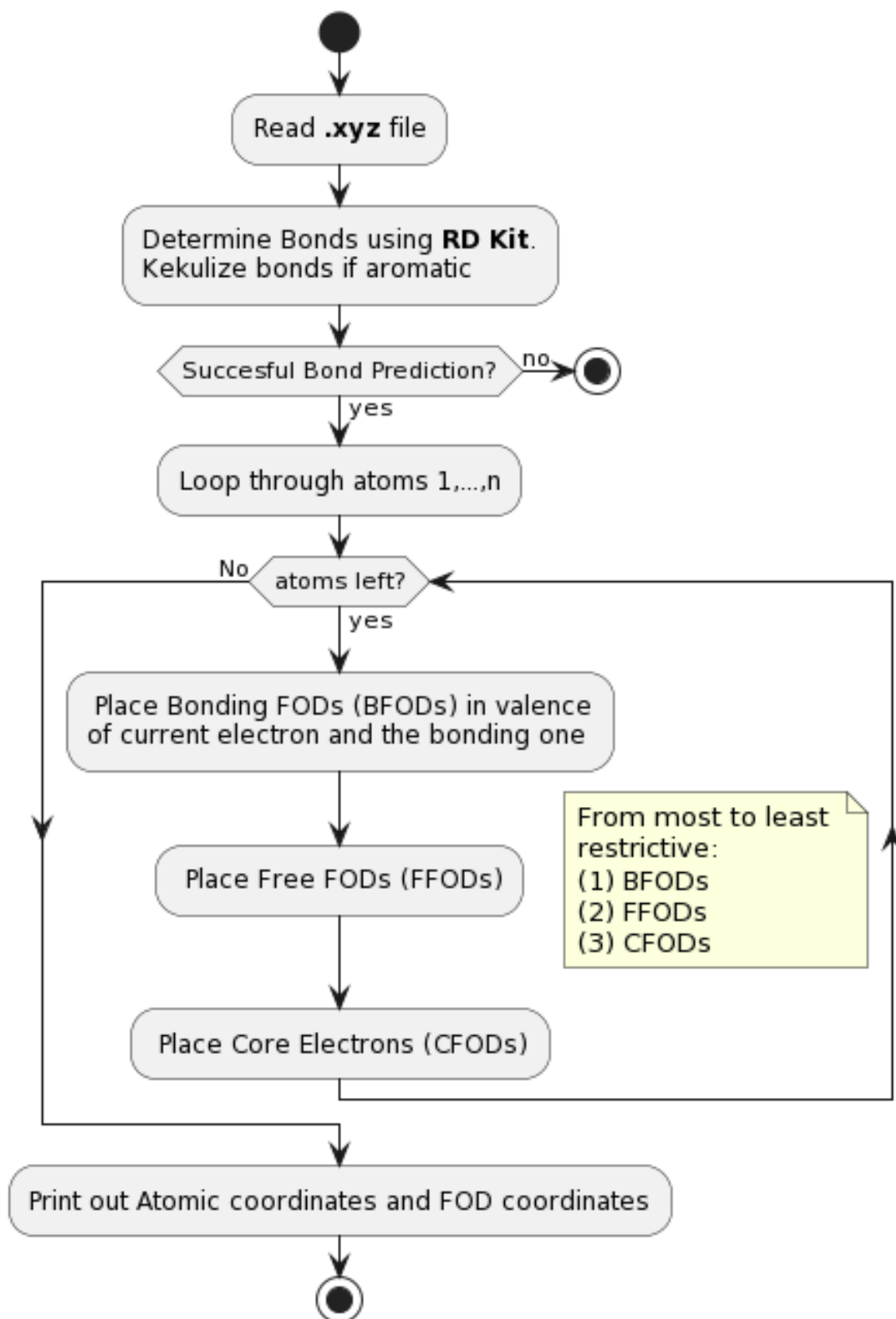
Figure 2: overview

A Heuristic-Based Approach to FOD Placement

- How can Heuristics help in computational problems?

Monoatomic Calculations

- Talk about *Dynamic Programming* and how monoatomic geometries could be pieced together in modular fashion (Lego-like).

Reparametrizing the FOD geometries

- sp3 shells stop being perfect tetrahedra and become irregular in the presence of other atoms.
- Describe how to parametrize FODs in irregular tetrahedra for the sp3 shells.

Implementation Details

- Describe code structure and use of object-oriented design
- Describe fundamental as seen in Figure 3

Molecule
mFile
mComment : String
mAtoms : List[Atoms]
mBonds : List[Bonds]
__LoadXYZ()
__RD_Bonds()
CheckStericity()
CalculateFODs()

Atom
mName : String
mPos : np.ndarray
ml : Integer
mZ : Integer
mPeriod : Integer
mGroup : Integer
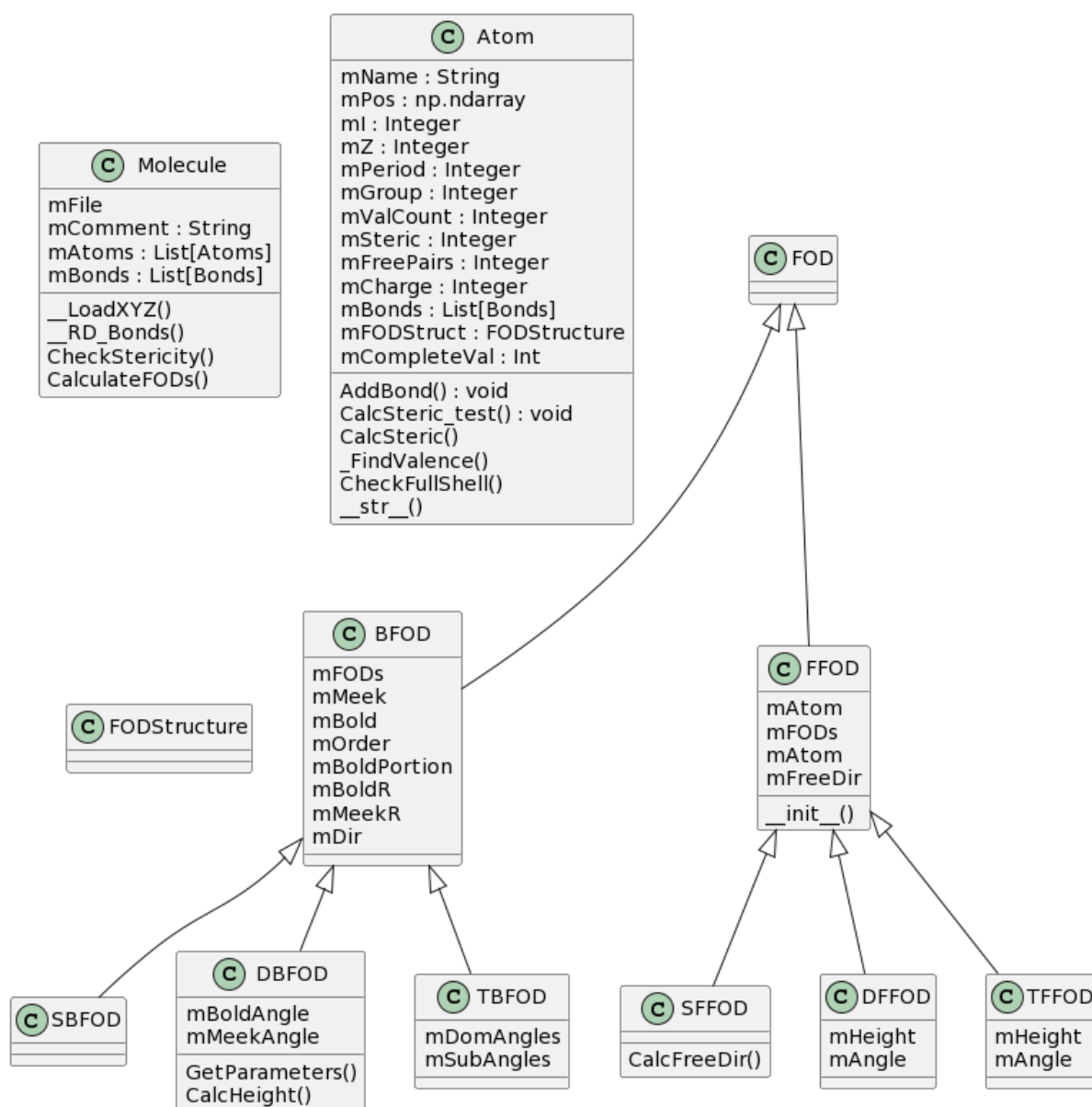mValCount : Integer
mSteric : Integer
mFreePairs : Integer
mCharge : Integer
mBonds : List[Bonds]
mFODStruct : FODStructure
mCompleteVal : Int
AddBond() : void
CalcSteric_test() : void
CalcSteric()
_FindValence()
CheckFullShell()
__str__()

FOD

FODStructure

BFOD
mFODs
mMeek
mBold
mOrder
mBoldPortion
mBoldR
mMeekR
mDir

FFOD
mAtom
mFODs
mAtom
mFreeDir
__init__()

SBFOD

DBFOD
mBoldAngle
mMeekAngle
GetParameters()
CalcHeight()

TBFOD
mDomAngles
mSubAngles

SFFOD
CalcFreeDir()

DFFOD
mHeight
mAngle

TFFOD
mHeight
mAngle

Figure 3: classes

Determination of FODs

- Describe the different determination heuristics for different types of FODs

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Bonding FODs (BFOD)

Core FODs (CFOD)

Free FODs (FFOD)

- Sample Diagram and calculation for Double-FFOD (DFFOD) Heuristic in Figure 4. The edge distance is applied to as a restriction.
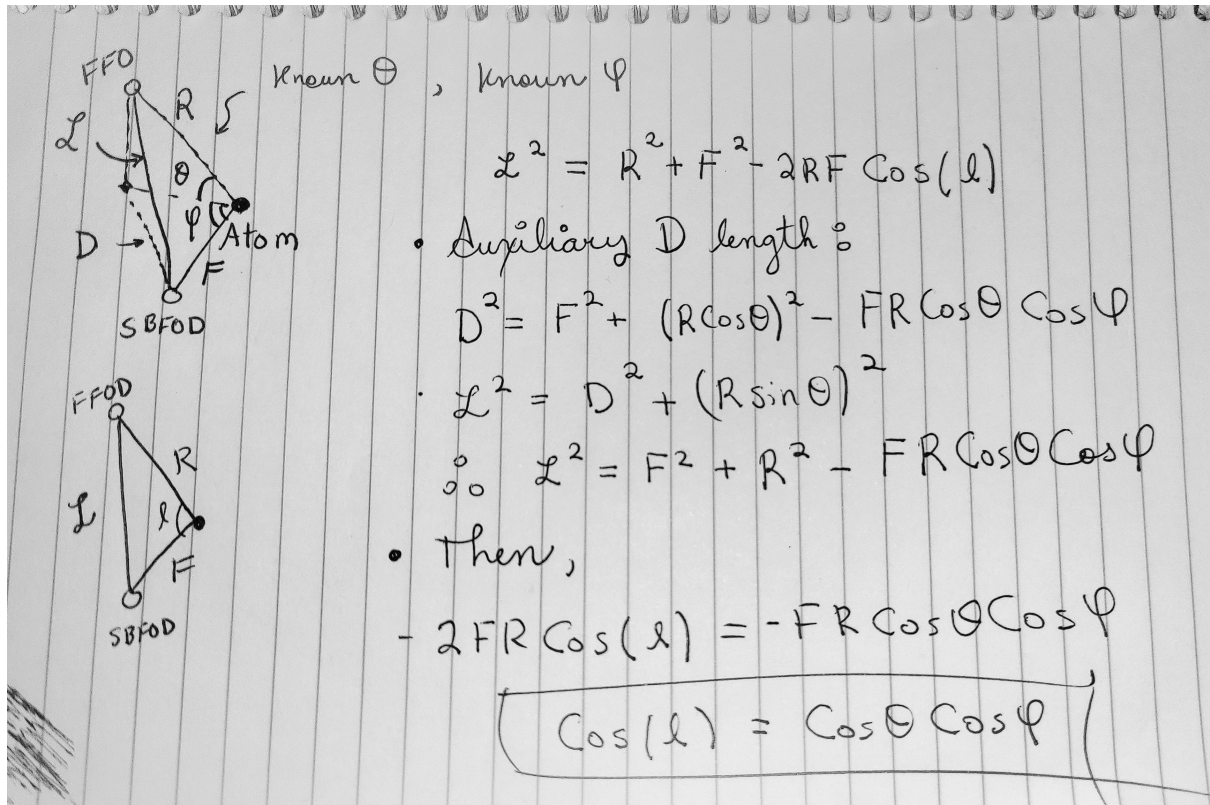

Figure 4: draft DFFOD

A Data-driven Approach to analyzing FODs

Reverse Determination of Parameters

This is the following implementation used for the reverse determination of parameters

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Algorithm 1: Reverse Parameter Determination Basic Sequence

Data: Relaxed FODs R_n

for *FOD in Predicted FODs* **do**

> Save closest R_n to FOD as R_{close};
>
> Initialize a new FOD with R_{close};

Free FODs (FFODs)   The free-direction, described in section XYZ, cannot be determined exactly. In order to best compare Free FODs in this parameter-based scheme, I propose using only an average direction formed from the average of all FFOD vectors and use an evaluation function. A cosine distance is too flat near its maximum, so a custom function can offer a more strict metric of our prediction

$$f(\theta) = 1 - 1/2 \tag{1}$$

Equation Equation **??** yields 1 when there at 0 degrees between the vectors, and 0 when there are 45 degrees between the vectors.

A database of compiled FOD Data

- No current database of FODs. Seeking to create a database
- **TODO!**

  - Design structure of database
  - Using FODLego, then FLOSIC, create optimized structures for a selection of molecules (scope?)

Validity of FOD Prediction

Explore the predictions done by FODLego

Comparison of Heuristic FODs to FLOSIC-Optimized FODs

- **TODO:**

  - Create scatter plots for different parameters described in the scheme of previous section.

Comparison to FOD-MC

Biasing Predictions after Sampling (?)

- – Assuming data follows certain trends, we can further modify the predictions used in FODLego. For example, the tightening of closed shells in heavier atoms in the presence of the next shell closed.

Discussion/Conclusions

Limitations

Assumptions

- Explore assumptions such as First neighbors are mainly considered in this scheme.

Automated Bonding Prediction

For Future Implementation

Extending modularity to metal FODs?

- Talk about possible parametrization of the *Triaugmented Triangular Prism* composed of 9 FODs.

Spin-Unpolarized Prediction