User Guide for ffr-ElectronicStructure.jl

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1 Introduction

 ${\tt ffr-ElectronicStructure.jl} \ \ is \ a \ collection \ of \ programs^1 \ for \ learning \ electronic \ structure \ calculations.$

2 Short introduction to Julia

```
H
type CircleT
  radius::Float64
end

H
type CircleT
  radius::Float64
end
```

3 Formulae

Plane wave basis $b_{\alpha}(\mathbf{r})$:

$$b_{\alpha}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} e^{\mathbf{G}_{\alpha} \cdot \mathbf{r}} \tag{1}$$

Structure factor:

$$S_I(\mathbf{G}) = \sum_{\mathbf{G}} e^{-\mathbf{G} \cdot \mathbf{X}_I} \tag{2}$$

¹or scripts