



Quantum Foca.jl

an application for quantum chemists



Quantum Foca.jl

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Seal = Foca

in english

in portuguese

it is inspired by another electronic structure package that has a name of a marine animal ...



Schroedinger equation

operator

$$\hat{H}\Psi = E\Psi \longrightarrow \text{eigenfunction}$$

eigenvalue

In computational chemistry, we solve this differential equation to get all the quantities we need!

Workflow



molecular integrals

Hartree-Fock, CCSD(T)



the fastest way to solve molecular integrals

Future ideas

- Mcmurchie-Davidson method
- Optimize geometries
- To support AtomsBase

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next release : July 30th

QuantumFoca.jl

OPEN ISSUES

20

BUILD

PASSING

COMMIT ACTIVITY

0/WEEK

DOI [10.5281/zenodo.6780563](https://doi.org/10.5281/zenodo.6780563)



