

# aiida-aimall: A Python package for automating workflows for AIMAll software

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## Software

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## Summary

Since its introduction by Richard Bader, the Quantum Theory of Atoms in Molecules (QTAIM) has become a useful tool for computational chemists. This Python package provides plugins for a common QTAIM software, AIMAll, for the AiiDA Python infrastructure. aiida-aimall is an essential tool for ensuring reproducible calculations, with full generation history. Workflows are also provided to interface AIMAll software with any quantum chemistry package that can be run through the command line, so long as it generates the input files required by AIMAll.

## Statement of need

aiida-aimall is a Python package based on the AiiDA (Talirz et al., 2020) infrastructure designed to assist users with generating inputs for AIMAll software (Keith, 2019). The goal of the AiiDA infrastructure are, in part, to ensure data provenance and calculation reproducibility. While aiida-aimall has been developed primarily for interface with Gaussian software outputs (Frisch et al., 2016), through modification of classes provided by aiida-gaussian (Eimre et al., 2023), a versatile workflow enabling interface with other quantum chemistry packages is also made available.

Through a variety of workflows that can start with Cartesian coordinates, or even with a SMILES string of a molecule, aiida-aimall provides a variety of use cases for automating and complex workflows. Additionally tools to ensure that computers are not overloaded through too many simultaneous processes are made available through classes of FromGroupSubmissionControllers from aiida-submission-controller to limit active processes.

## Features

aiida-aimall contains many different classes from aiida tailored to ensure ease of use of AIMAll calculations. Numerous features provided by aiida-aimall are provided in the documentation webpage hosted on ReadTheDocs. Select features are highlighted here.

Apart from the AimqbCalculation that provides the functionality, to run AIMAll calculations, a key feature is the AimqbParameters data type. The AimqbParameters datatype is a validator for AIMAll command line input. Command line parameters are to be provided as a dictionary, then AimqbParameters ensures that the parameters match options available for AIMAll software as defined on the software website, and that the correct data type is provided for each parameter. In this way, AimqbParameters verifies the provided input to AIMAll calculations prior to launch of the calculation.

Further, AiiDA workchains are provided to automate routine workflows associated with AIMAll calculations. The simplest workchain takes links a Gaussian calculation to an AIMAll calculation through a .wfx file produced by the Gaussian calculation. More complex workchains exist to

39 produce substituent parameters as defined by the authors in a series of publications. To not  
40 limit the usefulness of aiida-aimall to only users who use Gaussian software, an additional  
41 WorkChain is provided using aiida-shell to interface with any quantum chemistry package  
42 that can be run through the command line.

43 The last main contribution of aiida-aimall is through the definition of FromGroupSubmissionController  
44 from the aiida-submission-controller package. These controllers limit active processes  
45 and can be used together as demonstrated in (the example notebook) to automate the  
46 entire process of generating the author's substituent parameters for numerous inputs without  
47 overloading local or remote computers.

## 48 Mathematics

49 Single dollars (\$) are required for inline mathematics e.g.  $f(x) = e^{\pi/x}$

50 Double dollars make self-standing equations:

$$\Theta(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{else} \end{cases}$$

51 You can also use plain  $\LaTeX$  for equations

$$\hat{f}(\omega) = \int_{-\infty}^{\infty} f(x) e^{i\omega x} dx \quad (1)$$

52 and refer to [Equation 1](#) from text.

## 53 Citations

54 Citations to entries in paper.bib should be in [rMarkdown](#) format.

55 If you want to cite a software repository URL (e.g. something on GitHub without a preferred  
56 citation) then you can do it with the example BibTeX entry below for (?).

57 For a quick reference, the following citation commands can be used: - @author:2001 ->  
58 "Author et al. (2001)" - [@author:2001] -> "(Author et al., 2001)" - [@author1:2001;  
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## 60 Figures

61 Figures can be included like this: Caption for example figure. and referenced from text using  
62 [section](#) .

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