

功能概述

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一、注册与登陆

点击网站右上角【登陆】界面，如果是第一次访问，可以点击【注册】进行新用户注册，您可以通过邮箱注册或者绑定 GitHub 账户进行注册。

The image displays two side-by-side screenshots of a mobile application interface for '科学智能广场' (Science Intelligence Plaza). The left screenshot shows the login screen, and the right screenshot shows the registration screen.

Left Screenshot (Login):

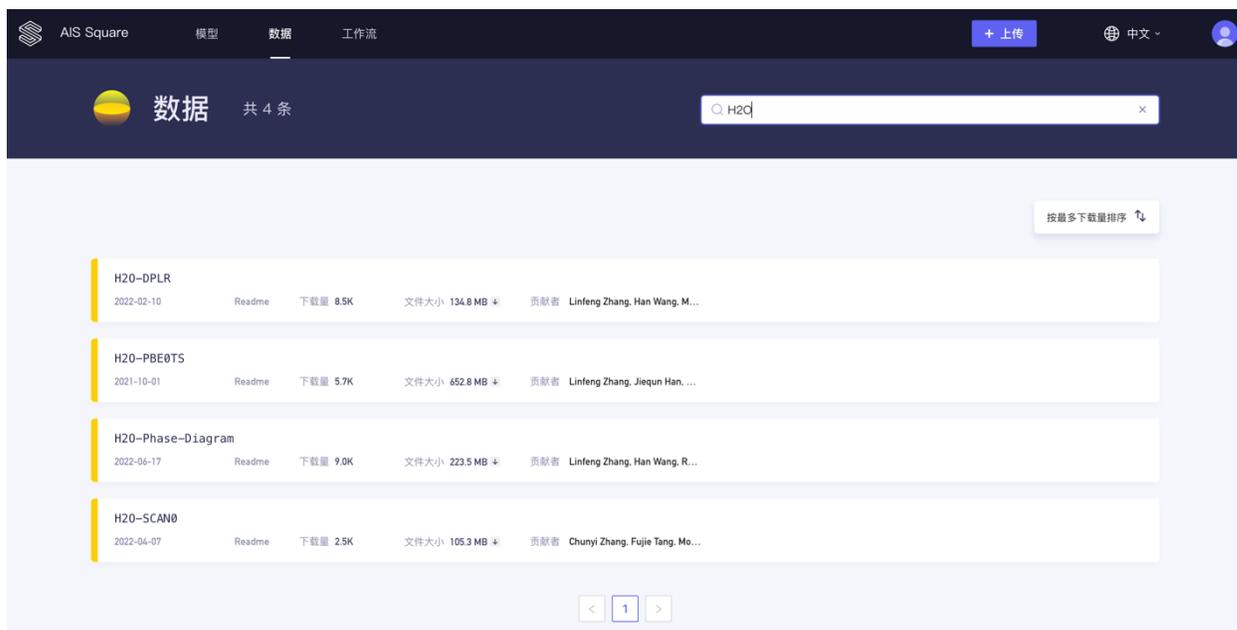
- Header: 科学智能广场 (Science Intelligence Plaza)
- Form fields: 邮箱 (Email) with value example@mail.com; 密码 (Password) with placeholder 6-18位长度 (6-18 characters) and a link 是否忘记密码 (Forgot password?).
- Buttons: 登录 (Login) in blue; Github 登录 (Login with GitHub) in white with a GitHub icon.
- Footer: 还没有账号? 现在注册 (No account? Register now).

Right Screenshot (Registration):

- Header: 注册账号 (Register Account)
- Form fields: Email (example@email.com); 验证码 (Verification code) with placeholder 验证码为6位 (Verification code is 6 digits) and a button 获取验证码 (Get verification code); 密码 (Password) with placeholder 6-18位长度 (6-18 characters) and a toggle icon; 再次输入密码 (Re-enter password) with placeholder 6-18位长度 (6-18 characters) and a toggle icon.
- Buttons: 注册 (Register) in blue; Github 注册 (Register with GitHub) in white with a GitHub icon.
- Text: 注册即代表同意 用户服务协议 和 隐私政策 (Registration represents agreement with User Service Agreement and Privacy Policy).
- Footer: 已有账号? 去登录 (Already have an account? Go to login).

二、检索、查看、下载条目

网站整体分为**数据**、**模型**和**工作流**三块内容，点击相应的模块进入条目检索界面，在检索框中输入对应的检索内容，检索结果会自动按照条目名称、详情内容和贡献者等检索范围进行展示。



点击对应的条目可以查看条目详情、贡献者、相关条目引用等信息，也包含了条目的格式和使用方式等内容。

Open_Catalyst_2020(OC20_Dataset)

更新时间 2022-11-24 下载量 15.1K 文件大小 4.1 GB 贡献者 Duo Zhang

Readme

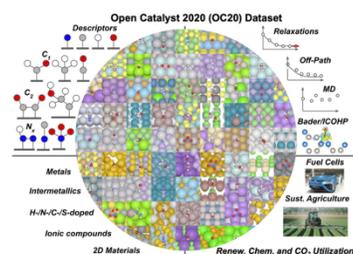


Figure 1. Adsorbates, materials, calculations, and impact areas of the OC20 dataset. Images are a random sample of the dataset.

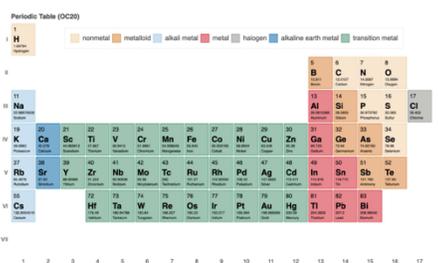


Figure 2. The elemental space of OC20 dataset.

引用
[datasets/Open_Catalyst_2022\(OC20_Dataset\)](#)

Introduction

Catalyst discovery and optimization is key to solving many societal and energy challenges including solar fuels synthesis, long-term energy storage, and renewable fertilizer production. A critical factor in building Machine Learning (ML) models is the data used for training. Much of the progress in applying ML in heterogeneous catalysis has been driven by increasingly large and diverse datasets of electronic structure calculations.

See [1] for more details on generation approach of OC20.

Data Format

The directory tree is as follows:

```
OC2M
-- train
-- -- [num_atom]
-- -- -- sys.xxxx
-- valid
-- -- [num_atom]
-- -- -- sys.xxxx
-- input.json
```

where each subdirectory ([num_atom]) consists of several systems sys.xxxx in DeepMD's mixed_type format, each of which contains num_atom atoms. input.json is a standard input script to train the DPA-1 model [3].

Each unit system sys.xxxx in mixed_type format usually has the following substructure:

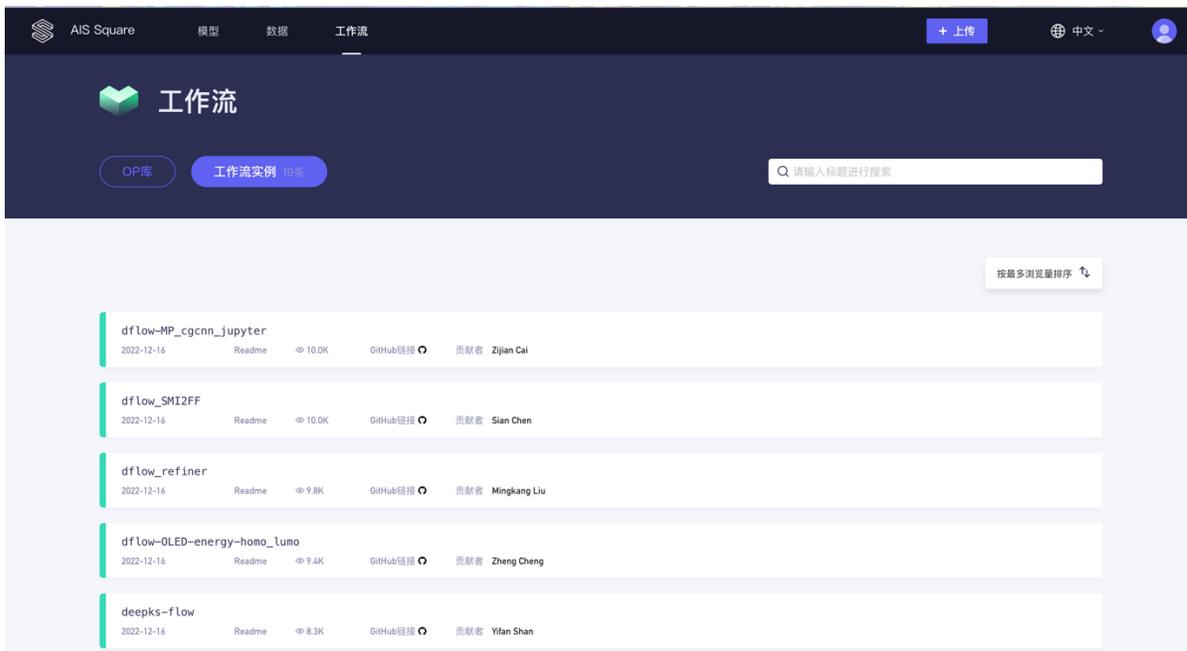
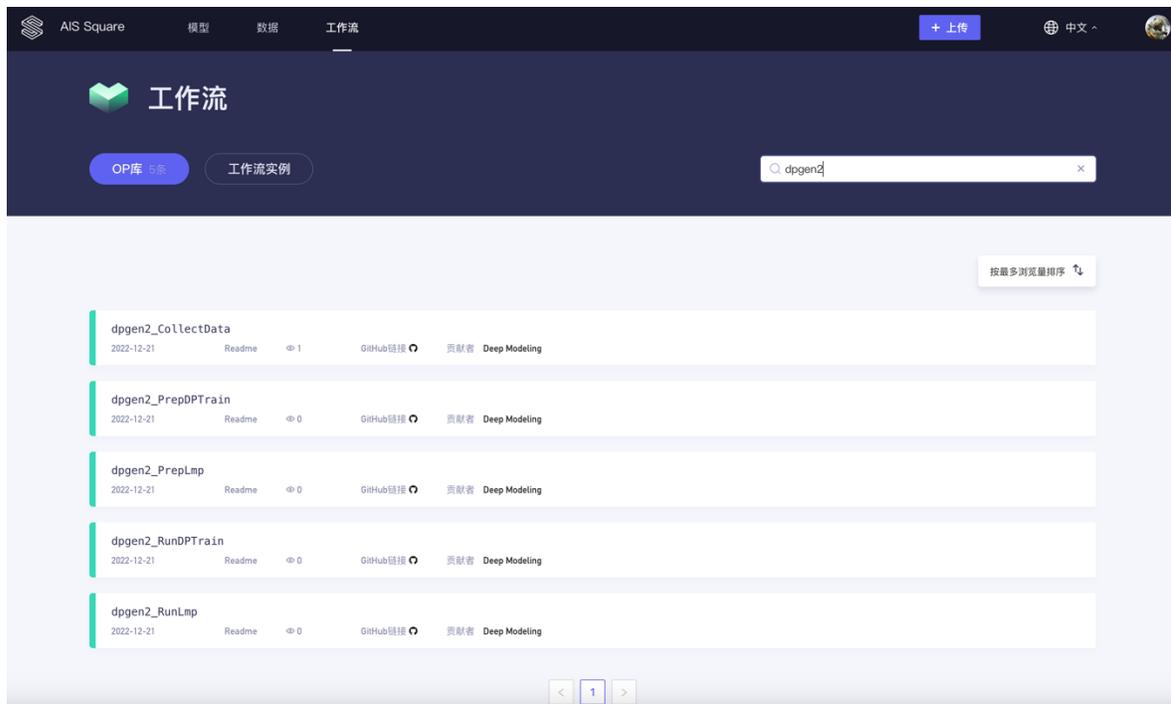
```
-- sys.xxxx
-- type_map.raw
-- type.raw
-- set.000/box.npy
-- set.000/coord.npy
-- set.000/energy.npy
-- set.000/force.npy
-- set.000/virial.npy
-- set.000/real_atom_types.npy
```

Format Description

| Name | Property | Raw file | Unit | Shape | Description |
|------|----------|----------|------|-------|-------------|
|------|----------|----------|------|-------|-------------|

对于数据和模型模块，还可以查看对应条目的文件大小和下载次数，在登陆的状态下，您可以点击下载按钮直接进行条目文件的下载。

在 workflow 模块，进一步分为 **OP 库** 和 **workflow 实例** 两部分。OP 库中主要包含单功能、可复用的 **dfLOW** 算子，方便开发者在构建自己 workflow 的时候直接使用；workflow 实例部分则包含了基于 **dfLOW** 实现的完整的工作流。



在 OP 库条目的详情页面，会详细介绍此 dflow 算子的功能和输入、输出格式，以及自动提取出来的 OP 源代码，方便开发者直接应用到自己的工作流开发中来，点击详情上方 GitHub 链接便可以直接跳转到此 OP 来源工作流的对应代码行。

The screenshot shows the AIS Square interface for the 'dpgen2_CollectData' operator. The page includes a header with navigation links (AIS Square, 模型, 数据, 工作流) and a '+ 上传' button. The main content area displays the operator's name, update time (2022-12-21), version (1), and a GitHub link. Below this is a 'Readme' section with the following details:

- Name:** dpgen2.op.collect_data.CollectData
- Input:**
 - name: (str) The name of this iteration. The data generated by this iteration will be place in a sub-directory of name.
 - labeled_data: (Artifact(List[Path])) The paths of labeled data generated by FP tasks of the current iteration.
 - iter_data: (Artifact(List[Path])) The data paths previous iterations.
- Output:**
 - iter_data: (Artifact(List[Path])) The data paths of previous and the current iteration data.
- Description:**

This OP is extracted from dpgen2 workflow.

This OP collect data scattered in directories given by ip['labeled_data'] in to one dpdata.Multisystems and store it in a directory named name. This directory is appended to the list iter_data.

On the right side, there is a '引用' (Cite) button with a link to 'workflows/instances/dpgen2'.

The bottom section of the screenshot shows the 'Description' and 'Source' (code) for the operator. The code is as follows:

```
# Inputs
name: str
type_map: typing.List[str]
labeled_data: Artifact(type=typing.List[pathlib.Path], optional=False, sub_path=True)
iter_data: Artifact(type=typing.List[pathlib.Path], optional=False, sub_path=True)

# Outputs
iter_data: Artifact(type=typing.List[pathlib.Path], optional=False, sub_path=True)

# Execute
@OP.exec_sign_check
def execute(
    self,
    ip: OPIO,
) -> OPIO:
    """Execute the OP. This OP collect data scattered in directories given by ip['labeled_data']
    in to one dpdata.Multisystems and store it in a directory named name. This directory is appended
    to the list iter_data.

    Parameters
    -----
    ip : dict
        Input dict with components:

        - name: (str) The name of this iteration. The data generated by this iteration will be place in a sub-directory
        - labeled_data: (Artifact(List[Path])) The paths of labeled data generated by FP tasks of the current iteration.
        - iter_data: (Artifact(List[Path])) The data paths previous iterations.

    Returns
```

在工作流实例中，点击条目可以查看详情介绍，点击详情上方 GitHub 链接也可以跳转到对应的 GitHub 仓库。

deepks-flow

更新时间 2022-12-21 8.1K GitHub链接 贡献者 Yifan Shan

Readme

Workflow which using dflow for DeePKS + ABACUS iteration

Introduction

I am glad to participate in the Hackathon activity in AI-assisted electronic structure calculations topic and have done this job with a minimum version, which I call deepks-flow.

This is a workflow which using dflow for DeePKS + ABACUS iteration. This iteration can build a bridge between expensive Quantum Mechanical Models and Machine Learning Potentials, which will significant decrease the cost of high-level *ab initio* calculation.

The diagram features the title "DeePKS + ABACUS" and the CNITECH logo. It includes the equation $E_{\text{DeePKS}} = E_{\text{baseline}} + E_{\delta}$. Below the equation, a blue arrow points to the text "高精度的数据作为计算目标". To the right, a 3D surface plot shows two energy surfaces: a blue one labeled "Original" and a green one labeled "Refined".

Running this project

Considering your python environment, maybe you should install some python package first.

```
pip install -r requirements.txt
```

We need to build the latest version of dflow. (This step added at 2022.9.1, maybe do not need do this after they upload the latest version to pip.)

```
pip install git+https://github.com/deepmodeling/dflow
```

Then, install the deepks2, which is a DeePKS + ABACUS iteration workflow using dflow.

```
pip install .
cd ./example/water_single_lda2pbe_abacus/iter
```

Before you submit the example, you may regist a Bohrium account and should modify some args around the end of base_args.yaml.

- scf_machine:program_id; train_machine:program_id; lebesgue_context_config:extra:program_id: input your program ID of your Bohrium program.
- username: input your Bohrium login account.
- password: input your Bohrium login password.
- upload_python_package: /path/to/deepks2 which you have just installed.

Now it's time to submit your workflow!

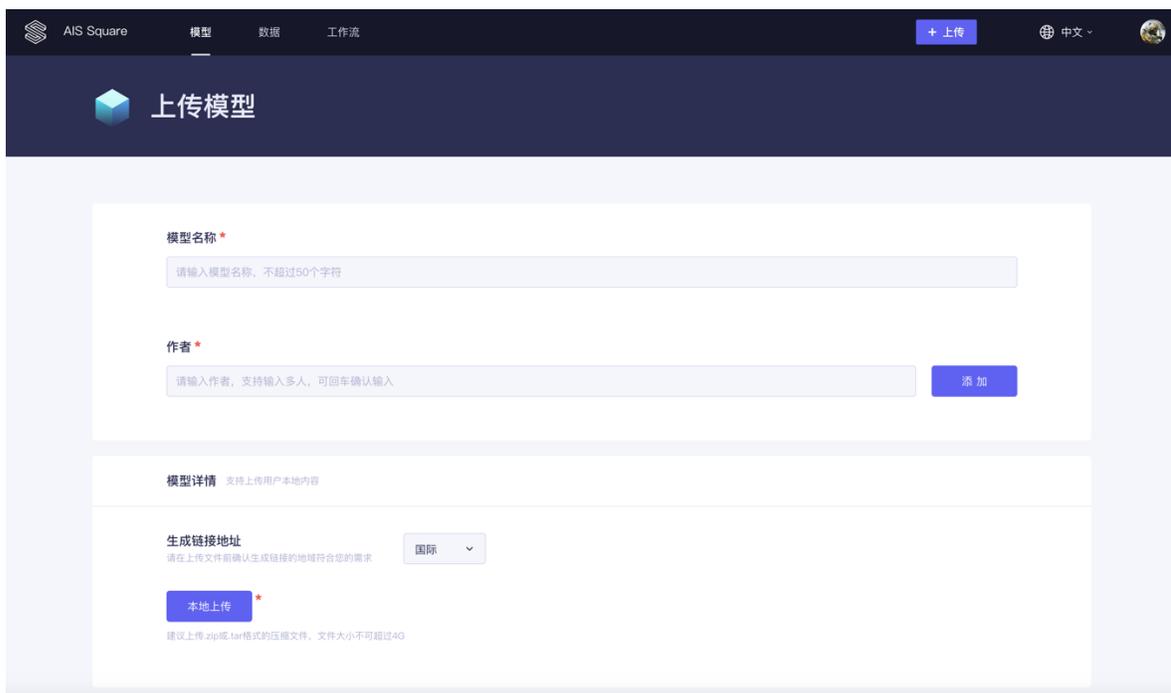
```
deepks2 iterate base_args.yaml
```

三、上传条目

在登陆状态下，您也可以分享您自己的数据、模型或者 workflow 条目到科学智能广场。点击右上角【上传】按钮，选择要上传的种类，便可以开始内容的上传流程。



在数据和模型的上传页面，您可以填入模型名称、作者等基本信息，并且选择本地文件进行上传。【注意：可根据您的网络速度，选择国际或者国内两种上传线路】



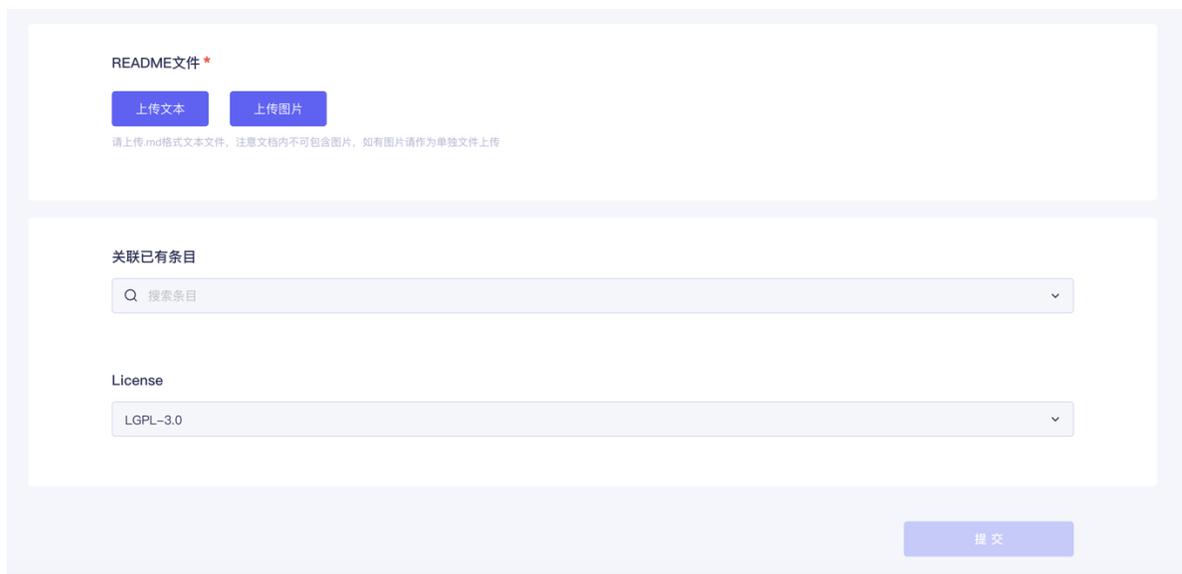
在 workflow 板块，您可以直接填入对应的 GitHub 仓库地址，而不需额外上传代码文件。



The screenshot shows the '上传工作流实例' (Upload Workflow Example) form. It includes the following fields and buttons:

- 工作流实例名称 *** (Workflow Example Name *): A text input field with a placeholder '请输入工作流实例名称, 不超过50个字符' (Please enter the workflow example name, no more than 50 characters).
- 作者 *** (Author *): A text input field with a placeholder '请输入作者, 支持输入多人, 可回车确认输入' (Please enter the author, supports multiple authors, press enter to confirm). A blue '添加' (Add) button is located to the right of the input field.
- GitHub地址 *** (GitHub Address *): A text input field with a placeholder '请输入GitHub地址' (Please enter the GitHub address).

完成上述步骤，或者在等待上传的同时，您可以在下方继续上传**文本文件**和**单张图片文件**，用来详细介绍此条目的内容，最终会作为条目详情界面的展示；在下方可以添加关联条目，将此条目和科学智能广场中已有的**任意条目**进行关联。



The screenshot shows the 'README文件' (README File) and '关联已有条目' (Associate Existing Items) sections of the form.

- README文件 *** (README File *): Two buttons, '上传文本' (Upload Text) and '上传图片' (Upload Image), are displayed. Below them is a note: '请上传.md格式文本文件, 注意文档内不可包含图片, 如有图片请作为单独文件上传' (Please upload .md format text files, note that images are not allowed in the document, if there are images, please upload them as separate files).
- 关联已有条目** (Associate Existing Items): A search input field with a magnifying glass icon and the placeholder '搜索条目' (Search items).
- License**: A dropdown menu currently showing 'LGPL-3.0'.

A blue '提交' (Submit) button is located at the bottom right of the form.

最后为了保护此条目的共享属性，您可以为此条目选择对应的 License，我们目前提供了如下图的四种可选 License：



如果有添加额外 License 的需要，请联系 aissquare@bjaisi.com。

等待上述步骤均完成之后，可以点击提交按钮，上传成功。

四、我的上传

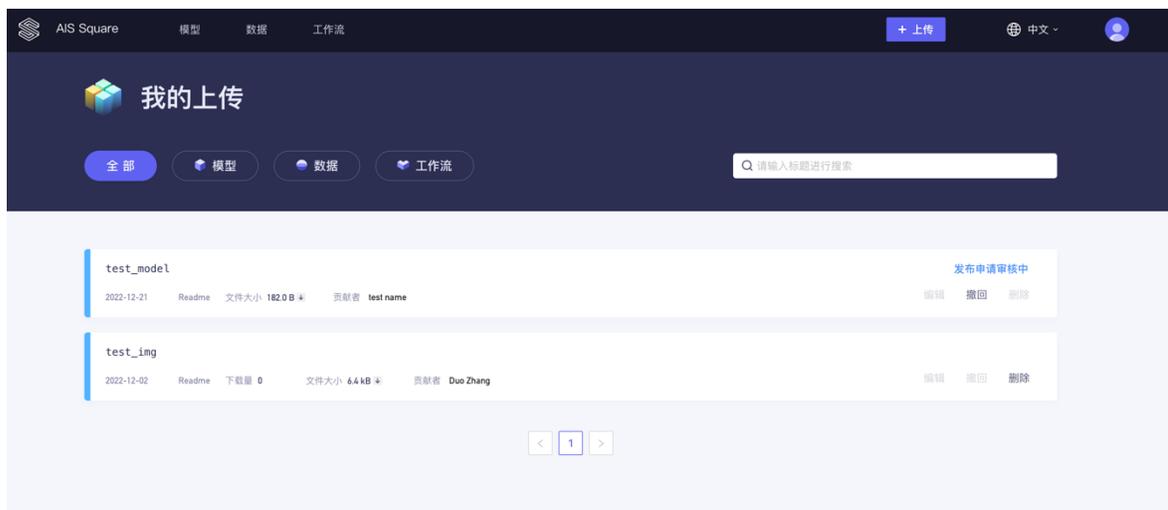
在完成上传之后，会自动跳转到【我的上传】界面，或者您也可以点击个人头像进入此界面。



在此界面中，将显示您所有已经提交成功的条目记录，并会显示当前条目的状态。共有以下几种条目状态：

- **【发布申请审核中】**：上传内容的 PR 已经提交成功，正在等待管理员的审核，此时可以点击条目查看详情；也可以点击**【撤回】**来取消本次上传，取消后会显示**【待提交】**状态。

- **【已发布】**：上传内容的 PR 已经通过审核，您上传的条目将会正式显示在科学智能广场；此时若点击**【删除】**按钮，将会再次将此记录从网站中完全删除。
- **【发布申请未通过】**：上传内容的 PR 未通过审核，您的邮箱将会收到消息，可以根据此消息，点击**【编辑】**来进一步对内容做出修改，重新上传。
- **【待提交】**：在**【发布申请审核中】**状态时，点击**【撤回】**来取消本次上传，取消后会显示此状态；此时您可以进行**【查看】**、**【编辑】**或者**【删除】**操作。
- **【删除申请审核中】**：在**【已发布】**状态下，若再次点击**【删除】**按钮并确定，将进入此状态，表明已经发布的内容正在等待管理员确认删除，删除成功将进入**【待提交】**状态。



您可以在此界面对已经上传或待上传的条目进行方便的管理。

更多功能正在开发中，敬请期待。