

Supporting Information

Electron density mapping of boron clusters via convolutional neural networks to augment structure prediction algorithms.

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Table 1: The Architecture of the Convolutional neural network.

Layers	Size
imageInputLayer	128,128,1
convolution2dLayer	3,8
batchNormalizationLayer	
reluLayer	
averagePooling2dLayer	2,3
convolution2dLayer	3,16
batchNormalizationLayer	
reluLayer	
averagePooling2dLayer	2,2
convolution2dLayer	3,32
batchNormalizationLayer	
reluLayer	
convolution2dLayer	3,32
batchNormalizationLayer	
reluLayer	
dropoutLayer(0.2)	
fullyConnectedLayer	10
regressionLayer	

**Microsoft Power automate script for cif file generation from
PDB files using the application VESTA:**

Get files in folder:

Retrieve the files in folder 'E:\.....' that match ".pdb" and move them into Files

For each CurrentItem in Files

Run application:

Run application 'CAVESTA-win64\VESTA-win64\VESTA.exe' with arguments CurrentItem

Wait 1 seconds

Move mouse:

Move mouse to 19, 52 (relative to Screen)

Send mouse click Send a Left click event

Move mouse:

Move mouse to 6, 305 (relative to Screen)

Send mouse click Send a Left click event

Wait 1 seconds

Send keys

Send the following keystrokes: (Return) to the active window

Wait 3 seconds

Send keys

Send the following keystrokes: (Control)((W)) to the active window

Wait 1 seconds

End

Microsoft Power automate script for Promolecule density generation from cif files using the application Crystal explorer:

Run application:

Run application 'C:\Program Files\Crystal Explorer CrystalExplorer.exe' and wait for it to load

Send keys:

Send the following keystrokes: '(Control)((O))' to the active window

Send keys:

Send the following keystrokes: 'C:\Users\minh\Desktop\4admpa_1.cif' to the active window

Send keys:

Send the following keystrokes: '{Return}' to the active window

Wait 1 seconds

Move mouse:

Move mouse to 40, 679 (relative to Screen)

Send mouse click:

Send a Right click event

Wait 1 seconds

Move mouse:

Move mouse to 141, 779 (relative to Screen)

Send mouse click:

Send a Left click event

Send keys:

Send the following keystrokes: '(Control)((G))' to the active window

Send keys:

Send the following keystrokes: '(Down)' to the active window

Send keys:

Send the following keystrokes: '(Down)' to the active window

Move mouse:

Move mouse to 1101, 731 (relative to Screen)

Send mouse click:

Send a Left click event

Move mouse:

Move mouse to 143, 61 (relative to Screen)

Send mouse click:

Send a Left click event

Move mouse:

Move mouse to 199, 637 (relative to Screen)

Send mouse click:
Send a Left click event

Move mouse:
Move mouse to 532, 666 (relative to Screen)

Send mouse click:
Send a Left click event

Wait 1 seconds

Send keys:
Send the following keystrokes: '(Return)' to the active window

Get files in folder:
Retrieve the files in folder 'E:\...' that match ".cif" and store them into Files

For each CurrentItem in Files

Send keys:
Send the following keystrokes: '{Control}{O}' to the active window

Set clipboard text:
Store the text CurrentItem into the clipboard

Send keys:
Send the following keystrokes: '{Control}{V}' to the active window

Send keys:
Send the following keystrokes: '(Return)' to the active window

Wait 1 seconds

Move mouse:
Move mouse to 40, 679 (relative to Screen)

Wait 1 seconds

Send mouse click:
Send a Right click event

Move mouse:
Move mouse to 141, 779 (relative to Screen)

Send mouse click:
Send a Left click event

Send keys:
Send the following keystrokes: '{Control} (\{G\})' to the active window

Send keys:
Send the following keystrokes: '(Return)' to the active window

Wait 40 seconds

Send keys:

Send the following keystrokes: '{Control}{S}' to the active window

Wait 1 seconds

Send keys:

Send the following keystrokes: '(Return)' to the active window

Wait 1 seconds

Move mouse:

Move mouse to 143, 61 (relative to Screen)

Send mouse click:

Send a Left click event

Move mouse:

Move mouse to 199, 637 (relative to Screen) in

Send mouse click:

Send a Left click event

Move mouse:

Move mouse to 532, 666 (relative to Screen)

Send mouse click:

Send a Left click event

Wait 1 seconds

Send keys:

Send the following keystrokes: '{Return}'
to the active window

End

The Crystal explorer generates cxs file containing coordinates of the surface of Promolecule density. We input the coordinate to matlab script which converts the 3d surface to 2d images. The code is given in the following link:

[pointcloud2image\(x,y,z,numr,numc \) - File Exchange - MATLAB Central \(mathworks.com\)](#)

The images so obtained are stored in Matlab 3D array:

```
f=dir('* .png');
files={f.name};
for k=1:numel(files)
    train{k}=imread(files{k});
    train{k}=imresize(test{k},[128 128]);
end
```

The output variable are the corresponding energies obtained from Gaussian calculation and they are stored as Y variable. The training of the neural network is done by the following command:

```
net = trainNetwork(XTrain,YTrain,layers,options);
```

We have utilized the layers specified in table 1 of ESI.

The options are as followed:

```
options = trainingOptions('sgdm', ...
'MaxEpochs',150, ...
'InitialLearnRate',1e-5, ...
'LearnRateSchedule','piecewise', ...
'LearnRateDropFactor',0.1, ...
'LearnRateDropPeriod',20, ...
'Shuffle','every-epoch', ...
'ValidationData',{val,valY}, ...
'Plots','training-progress', ...
'Verbose',false);
```

Useful shell script and the neural network model itself is given in the following github link:

<https://github.com/314111953/Featureless-learning-using-Promolecular-Density/tree/main>