

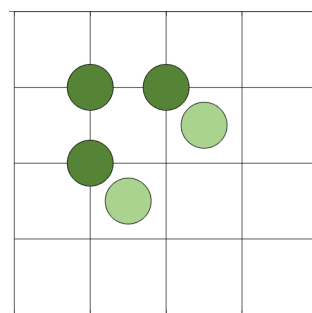
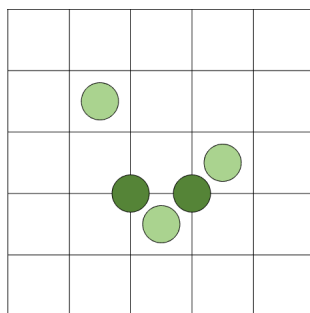


WASHINGTON STATE  
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# Using AMALGM to build Lattice Gas Cluster Expansions

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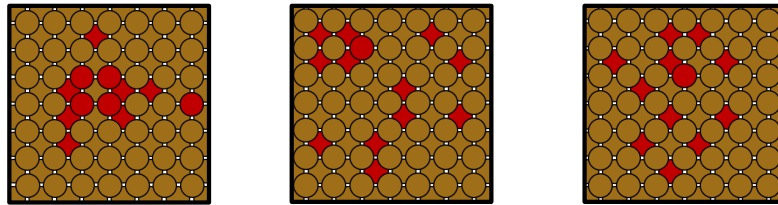




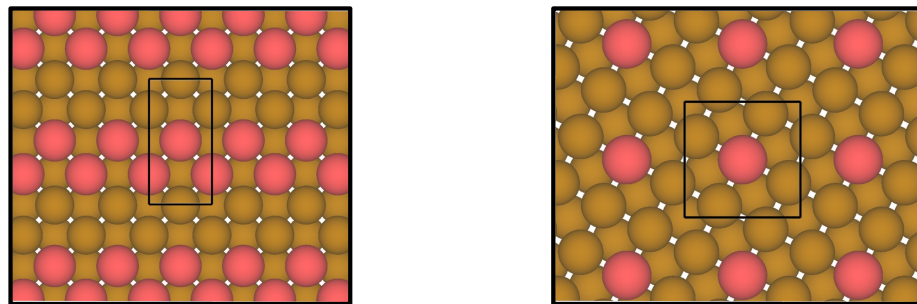
## Cluster Expansions

Used to study systems that exhibit substitutional disorder

- Sites on the surface can be occupied by more than one atom
  - Bimetallic systems
- Multiple configuration with different properties



- Function representing the configuration dependence of the system's energy - LG CE
- AMALGM to build LG CEs
  - Pd-Fe(100) bimetallic surface





## Running Directory

<https://github.com/gbcollinge/AMALGM>

The screenshot shows a file explorer window with the 'Current Folder' set to 'configs'. The file list includes:

- configs
- LG\_ECIs
- new\_configs
- circles.m
- CV\_calc\_v3.m
- nmultichoosek.m
- ANALYZE\_CE\_v4.m
- clean\_configs.m
- CONSTRUCT\_CE\_v4\_4.m
- COUNTS\_GEN\_v7\_4.m
- INTERACTION\_GEN\_v3\_2.m
- overnight\_CE.m

The 'configs' subdirectory is expanded, showing a list of files including 'atat0', 'atat1', 'atat10', 'atat100', 'atat101', 'atat1017', 'atat10185', 'atat102', 'atat1022', 'atat104', 'atat1049', 'atat105', 'atat1056', and 'atat106'. A callout box points to the file 'atat100' and displays its contents as a matrix:

-2	1	
2	1	
-0	0	2
-1	1	2
0	1	2
-.10591780E+03		



## Interactions in AMALGM

```
maxNbody= 2;
```

Maximum multi-body interactions for the LG CE

```
##### BOOK KEEPING, PLEASE DON'T TOUCH #####
vecbody = [ones(1,maxNbody)*maxNbody maxNbody];
Rmax = zeros(vecbody);
##### OKAY DONE, CONTINUE #####

% User defined maximum interaction distances "Rmax" in units of
% natural unit vectors. Each matrix (e.g. Rmax(:,2)) corresponds to a
% n-body interaction (e.g. 2 body interaction). Each row and column
% correspond to each site type (so if there are 3 site TYPES, these
% will be 3 x 3 symmetric matrices. Each element corresponds to
% interactions between the types designated by the row and column. For
% example, if there are 3 site types (1, 2, and 3), Rmax(:,3) contains
% the maximum site distances (or "cluster sizes") for 3-body interactions
% and Rmax(1,3,3) is the maximum 3-body site distance between sites
% 1 and 3 (corresponding to the sites entered above). If you want (say) 4
% body interactions between site 1 and itself (Rmax(1,1,4)) but not between
% site 1 and 2, just enter "0" for that entry (i.e. Rmax(1,2,4) = 0).
```

```
Rmax(1,1,2) = 5;
Rmax(2,2,2) = 5;
Rmax(1,2,2) = 5;
```

Specifying 2-body interaction

```
%Rmax(1,1,1,::,3) = 3.5;
%Rmax(2,2,2,::,3) = 3.5;
%Rmax(1,2,2,::,3) = 3.5;
%Rmax(1,1,2,::,3) = 3.5;
```

```
%Rmax(1,1,1,1,::,4) = 3;
%Rmax(2,2,2,2,::,4) = 3;
%Rmax(1,2,2,2,::,4) = 3;
%Rmax(1,1,2,2,::,4) = 3;
```

```
%Rmax(1,1,1,1,1,5) = 2.5;
%Rmax(2,2,2,2,2,5) = 2.5;
%Rmax(1,2,2,2,2,5) = 2.5;
%Rmax(1,1,2,2,2,5) = 2.5;
```

In INTERACTIONS\_GEN\_vx.m and COUNTS\_GEN\_vx.m



## First time running

1. Run INTERACTION\_GEN\_v3\_2.m
2. Run COUNTS\_GEN\_v4\_4.m

### Command Window

Working...

-----  
Directory "new\_configs" has been created...  
...checking if a LG model has been provided...  
"LG\_ECIs.txt" not found.  
Would you like this script to simply move any new structures  
found in folder "new\_configs" to folder "configs"?

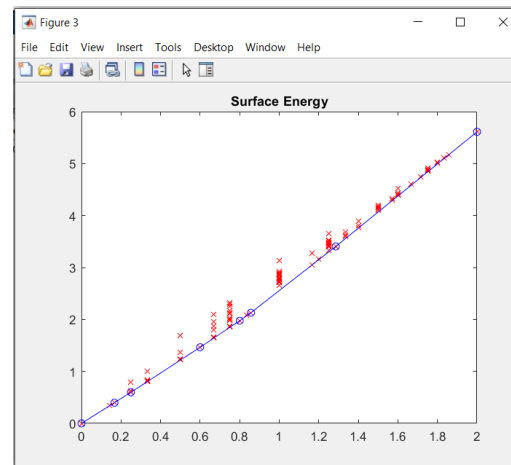
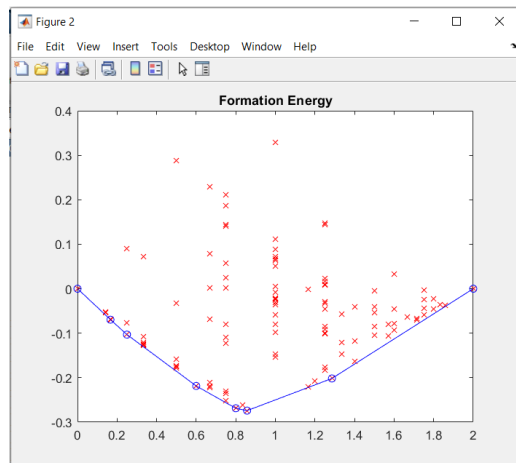
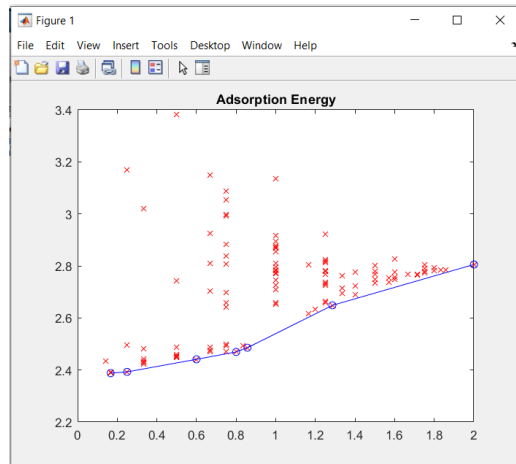
fx Enter "1" (yes) or "0" (no): 0

### Current Folder

	Name
+	configs
	LG_ECIs
	new_configs
	circles.m
	CV_calc_v3.m
	nmultichoosek.m
	ANALYZE_CE_v4.m
	clean_configs.m
	CONSTRUCT_CE_v4_4.m
②	COUNTS_GEN_v7_4.m
①	INTERACTION_GEN_v3_2.m
	overnight_CE.m



## First time running



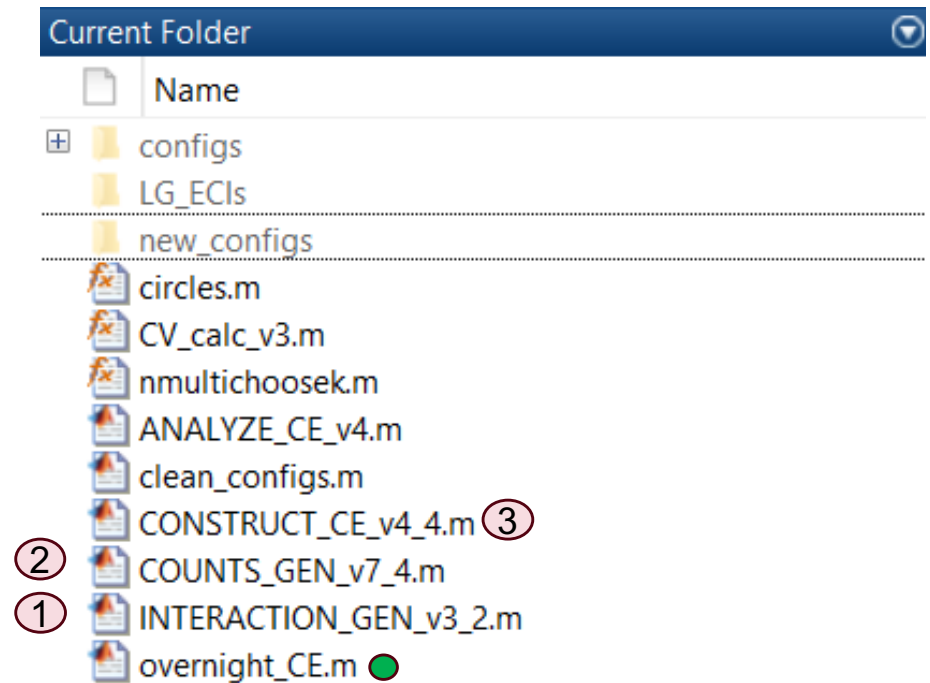
Current Folder

Name
configs
LG_ECIs
MC_POSITIONS
new_configs
SURF_ENERGY
circles.m
CV_calc_v3.m
nmultichoosek.m
ANALYZE_CE_v4.m
clean_configs.m
CONSTRUCT_CE_v4_4.m
COUNTS_GEN_v7_4.m
INTERACTION_GEN_v3_2.m
overnight_CE.m
Adsorption_Energy.png
Formation_Energy.png
Surface_Energy.png
CLUSTER_POSITIONS.txt
COUNTS_MATRIX.txt
COVERAGES.txt
INTERACTIONS.txt
NORMALIZED_MATRIX.txt
zero_energy.txt



## First time running

1. Run INTERACTION\_GEN\_v3\_2.m
2. Run COUNTS\_GEN\_v7\_4.m
3. Run CONSTRUCT\_CE\_v4\_4.m
  - Run Overnight\_CE.m





## Output after CONSTRUCT\_CE Run

The algorithm has found a local minimum!  
No further cluster additions or removals lower the CV score

The final CE is:

1	2	6	8	9	11	18	20	27
---	---	---	---	---	----	----	----	----

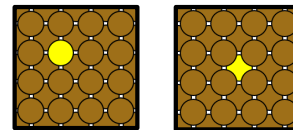
→ Copy to use in  
ANAYLZE\_CE

Its CV score is: 0.0356551 eV/site  
Its standard deviation is: 0.035625 eV/site  
The RMSE of the final fit is: 0.0264875 eV/site  
The LG ECI for this CE are:

3.1012
2.4024
-0.017756
-0.080761
0.0349
0.039307
0.077126
-0.046214
0.066299

This CE corresponds to the following interactions:

1	0	0
2	0	0
1	1	5
1	1	9
1	1	10
1	1	16
1	2	4.5
1	2	8.5
2	2	1







## Running ANALYZE\_CE

### Run COUNTS\_GEN

```
Directory "new_configs" has been created...
...checking if a LG model has been provided...
"LG_ECIs.txt" found.
This script will calculate the external-CV score for any new configurations
found in folder "new_configs".
Do you want to move any non-problematic structures found in new_configs to folder "configs"?

Enter "1" (yes) or "0" (no): 0
Do you want to move any problematic structures found in new_configs to folder "prob_configs"?

Enter "1" (yes) or "0" (no): 0|
```

### Run ANALYZE\_CE

```
% If you'd like to specify that certain clusters be added at the start (no
% guarantee the algorithm won't remove them, mind you) add them here. Note:
% if you don't want ANY starting clusters, just delete the numbers and
% leave an empty set...do not comment this out.

CE = [1 2 6 8 9 11 18 20 27];

% Do you want to check for unrepresented clusters? ("1" = yes, "0" = no)

check_flag = 0;
|
% Do you want to plot all the clusters found?
% "0" = no; "1" = yes; "2" = plot AND save to a png file

plot_clusters = 2;
```



## Output after ANAYLZE\_CE Run

Its CV score is: 0.0290251 eV/site

Its standard deviation is: 0.0289702 eV/site

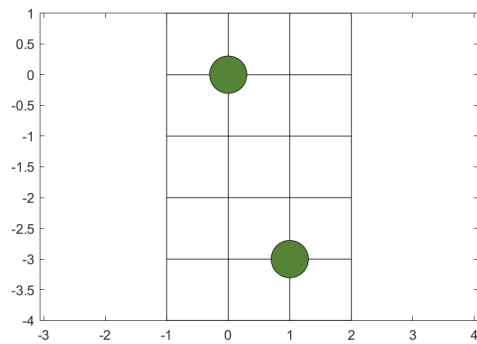
-----  
-----

Ready to plot the clusters in the CE.

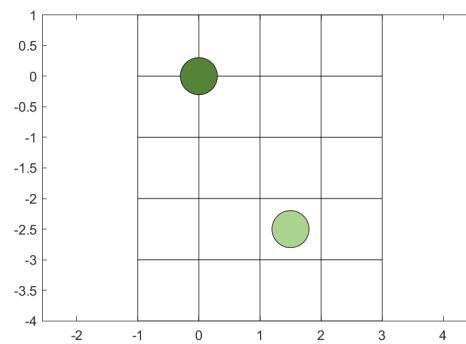
Do you want to plot the clusters with "inf" EIC?

"no" = "0" ; "yes" = "1"

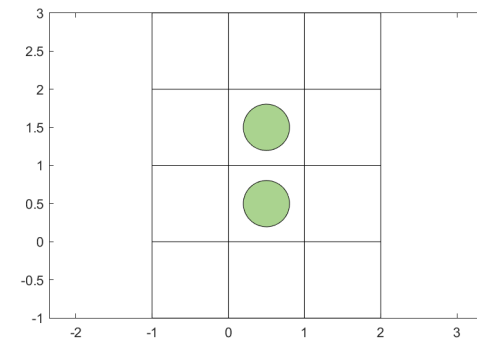
Choice: 0|



Cluster 9  
FCI (eV) = 0.024861



Cluster 20  
FCI (eV) = -0.045201





Cluster 27  
FCI (eV) = 0.091464



## Output after ANAYLZE\_CE Run

Cluster#	ECI	ECI_error	percent_error	confidence intervals (eV)	
1	3.0971	0.017586	0.56783	0.022751	
2	2.3628	0.016272	0.68868	0.021125	
6	-0.01827	0.0071925	39.368	0.0078976	
8	-0.060446	0.016022	26.507	0.016969	
9	0.024861	0.00885	35.598	0.007351	
11	0.037844	0.016955	44.802	0.013319	
18	0.080666	0.016305	20.213	0.027306	
20	-0.045201	0.011057	24.462	0.014617	
27	0.091464	0.011429	12.496	0.011785	

 LG\_ECIs.txt  
 LG\_Model.txt

Structure	Coverage	Ads_Energy	Surf_Energy
'atat0'	0	0	0
'atat1751'	0.16667	2.3879	0.39798
'atat133'	0.25	2.3927	0.59817
'atat1017'	0.6	2.4411	1.4646
'atat1022'	0.8	2.4694	1.9756
'atat13432'	0.85714	2.4857	2.1306
'atat12510'	1.2857	2.6485	3.4052
'atat1'	2	2.8054	5.6108



## Getting External CV score

Populate the new\_configs directory  
and run COUNTS\_GEN again

Only nonequivalent configurations  
will be considered

External CV score and residuals  
(surface energy) for the  
nonequivalent configurations

```
The external-CV score is 0.0238366 eV/site
The standard deviation of the residuals is 0.0238306 eV/site
The external-CV deviation is 0.0266577 eV/site
The residuals are:
atat2131  0.0129982
atat214   0.00687
atat2148  0.00208467
atat215   0.025992
atat2154  -0.0100363
atat216   -0.0228998
atat2197  0.0292438
atat22    -0.006724
atat221   -0.0115485
atat222   0.028059
atat224   0.02939
atat2252  -0.0023865
atat227   -0.0023205
atat228   0.00274975
atat229   0.0130648
atat23    -0.0335013
atat230   0.044693
atat232   0.0102515
atat234   -0.0380215
atat235   0.0379005
atat236   -0.014876
atat237   -0.0155385
atat238   -0.020218
atat239   -0.0337525
atat24    -0.0300913
atat240   -0.0405525
atat2411  0.00602283
atat2412  0.0262022
atat2417  0.0463197
```



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**THANK YOU**

