Computational Model and Characterization of Stacking Faults in ZIF-8 Polymorphs

Supporting Information

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Additional ZIF-8 polymorphs emphasizing the extended defect

Figure S1. FAU-ZIF8 without (top) and with (bottom) a stacking fault

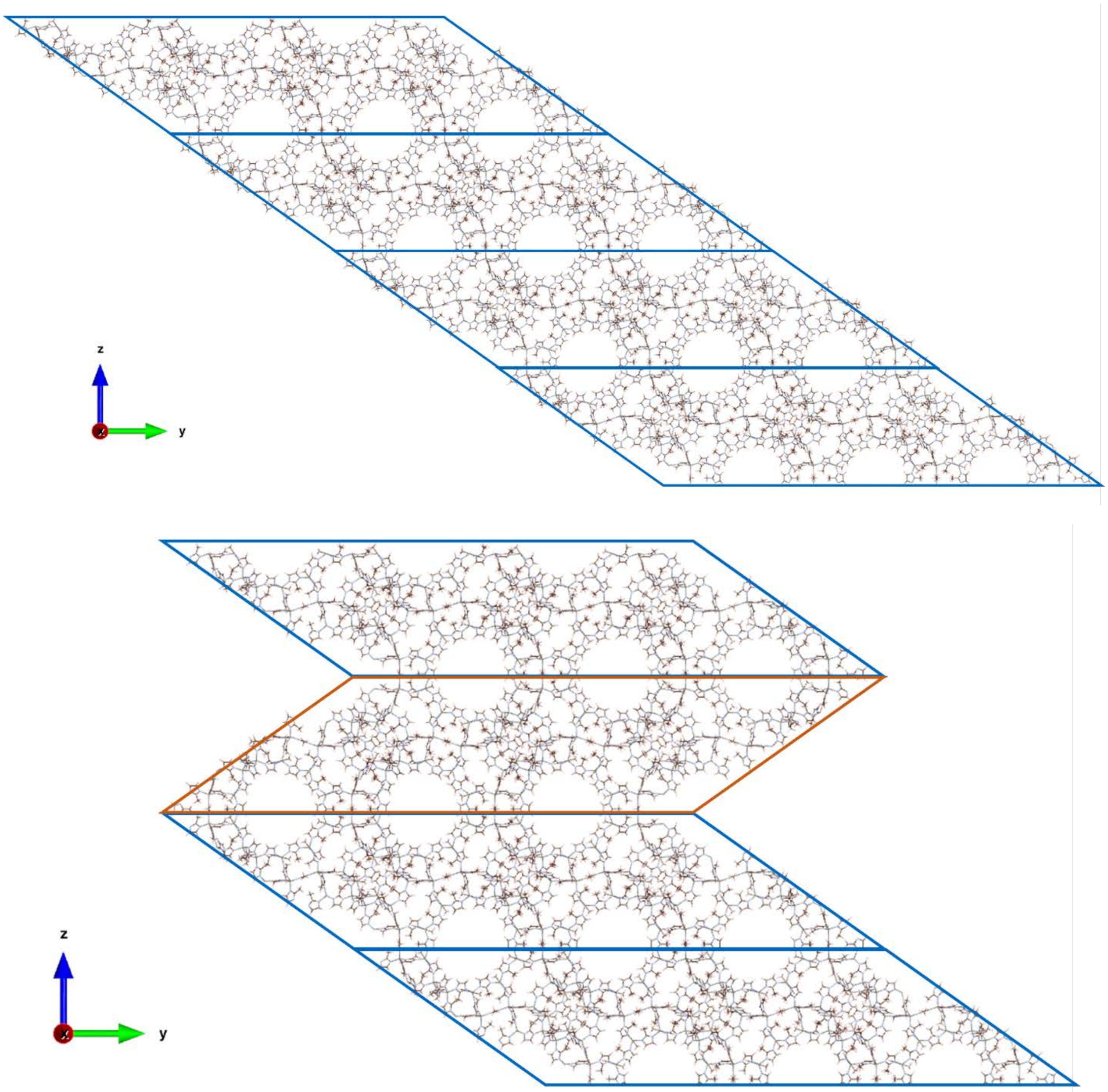


Figure S2. CDO-ZIF8 without (left) and with (right) a stacking fault

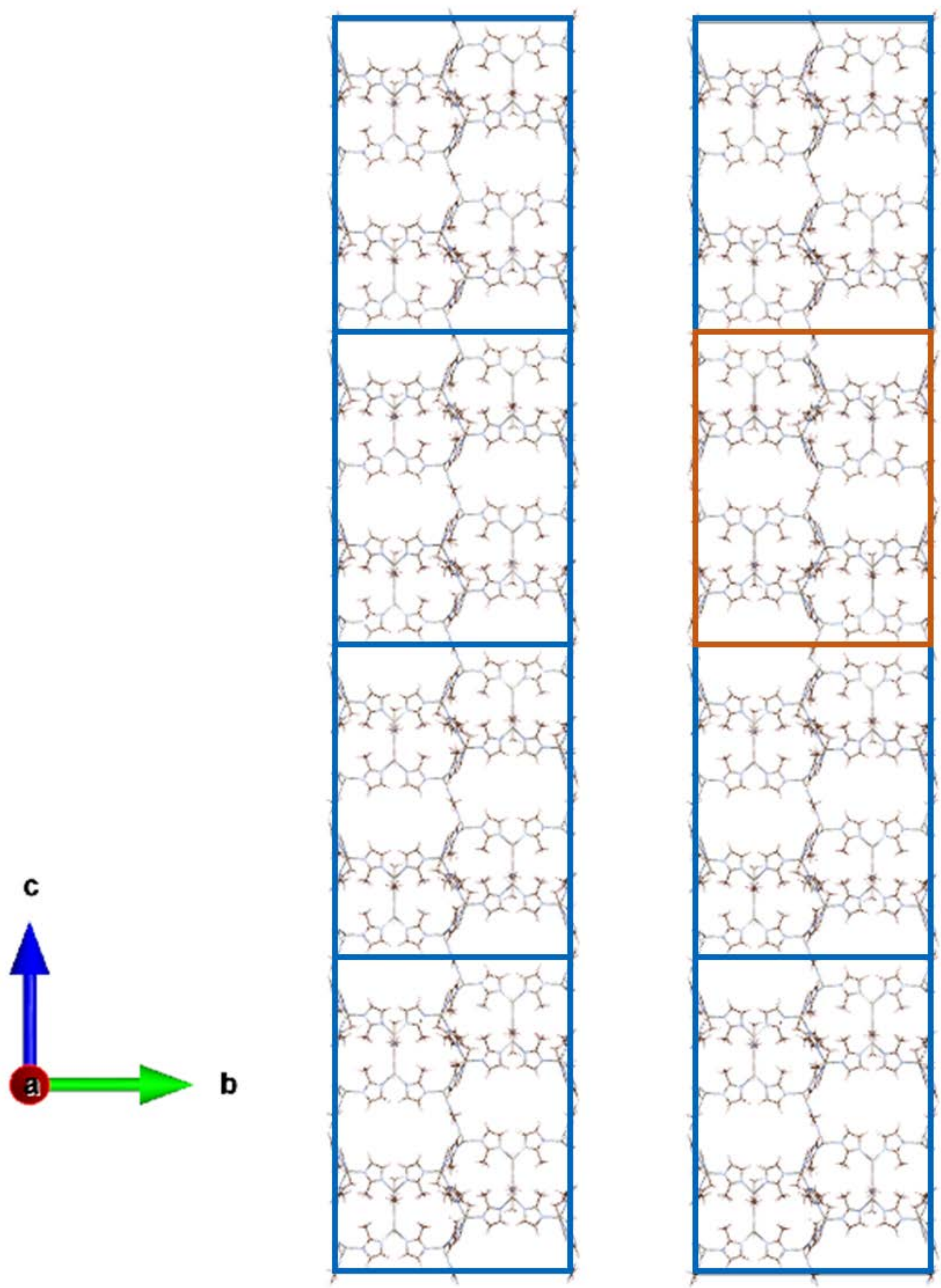


Figure S3. RTH-ZIF8 without (top) and with (bottom) a stacking fault

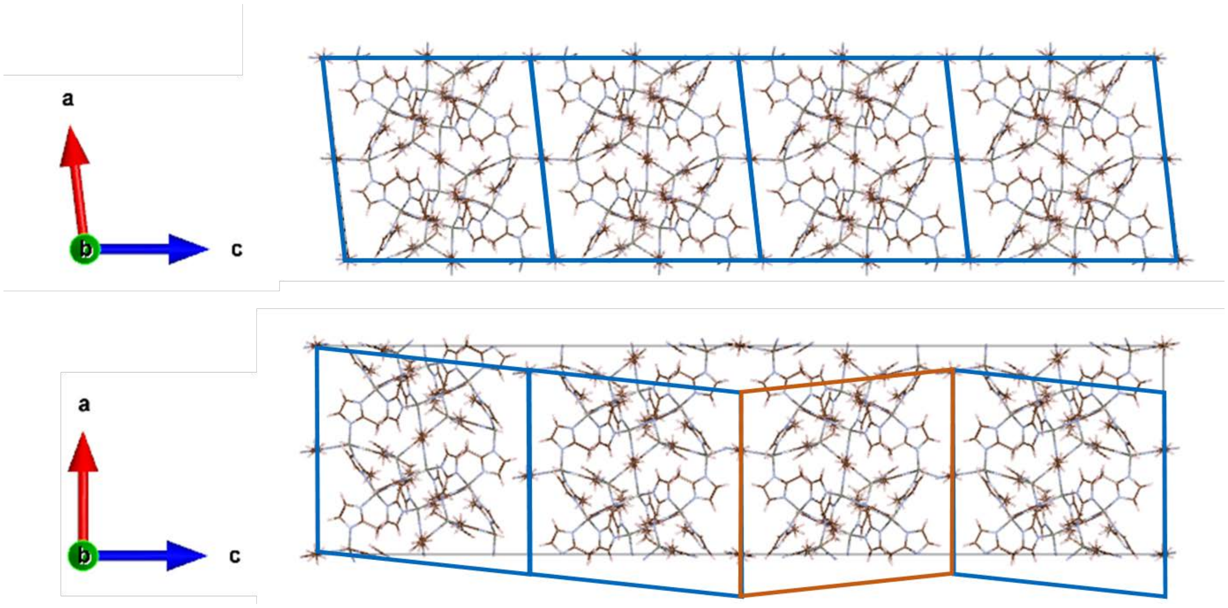
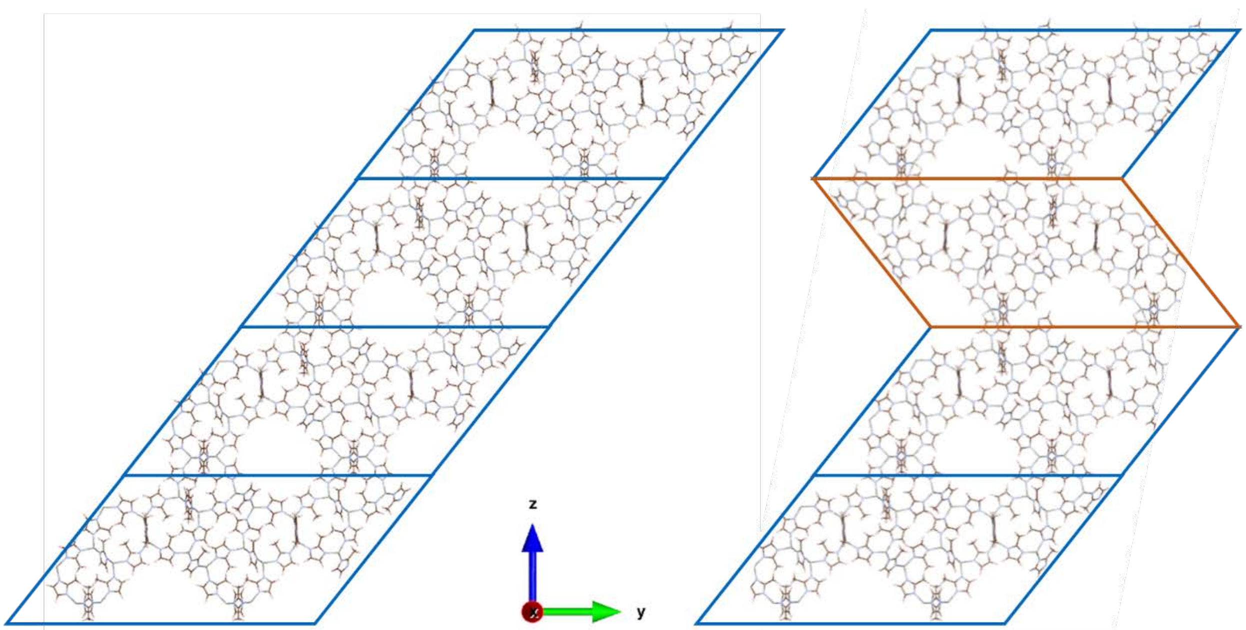
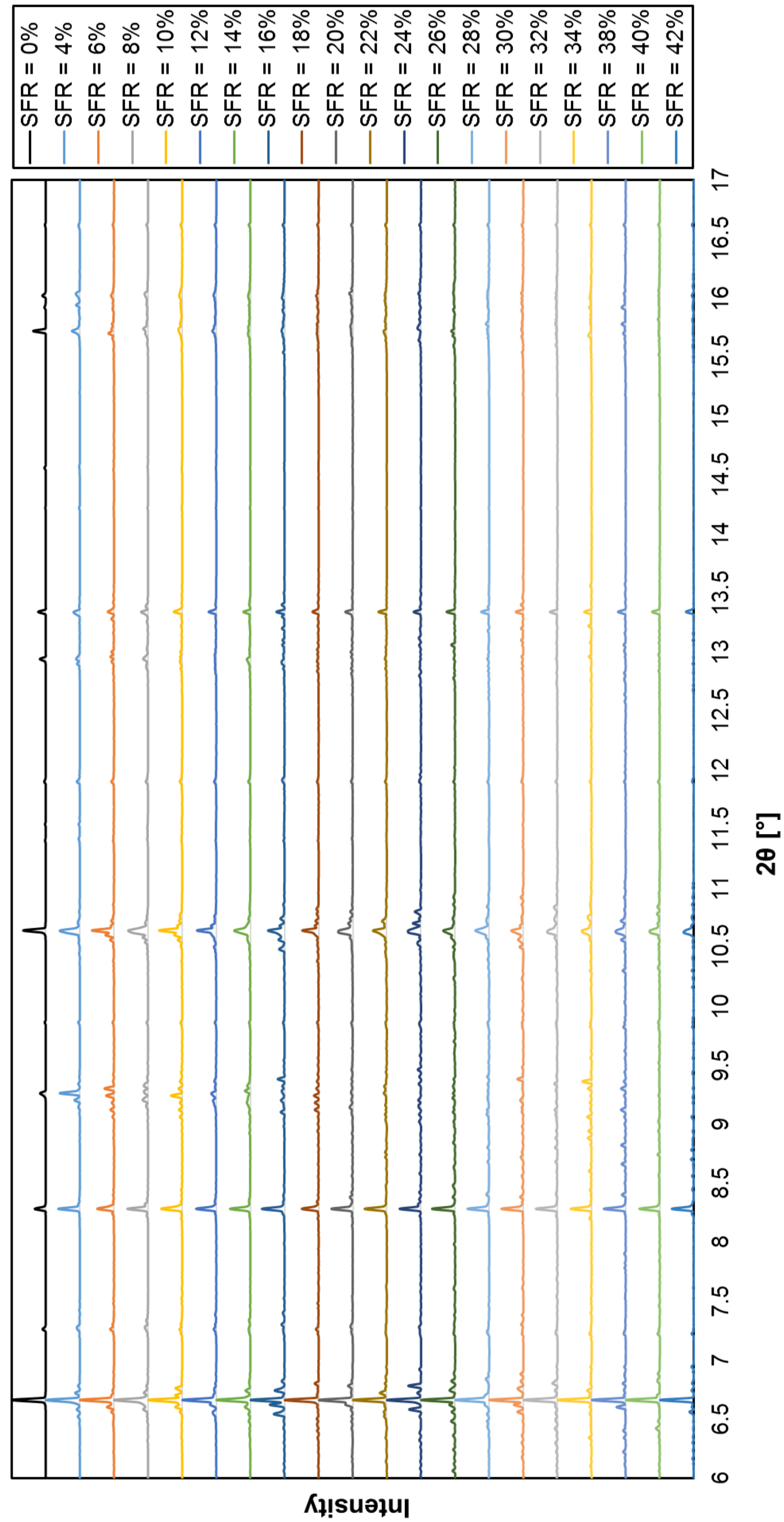


Figure S4. TON-ZIF8 without (left) and with (right) a stacking fault



Simulated CHA-ZIF8 X-ray diffraction patterns of increasing stacking fault ratio (SFR)

Figure S5. XRD spectra averaged over ten structures for each SFR


SFR = 0%
SFR = 4%
SFR = 6%
SFR = 8%
SFR = 10%
SFR = 12%
SFR = 14%
SFR = 16%
SFR = 18%
SFR = 20%
SFR = 22%
SFR = 24%
SFR = 26%
SFR = 28%
SFR = 30%
SFR = 32%
SFR = 34%
SFR = 38%
SFR = 40%
SFR = 42%
Intensity
2θ [°]
6
6.5
7
7.5
8
8.5
9
9.5
10
10.5
11
11.5
12
12.5
13
13.5
14
14.5
15
15.5
16
16.5
17

Principal components and additional correlations

Coefficients of principal component analysis (PCA) for peak intensity and area are listed in Tables S1 and S2, representing the correlation of the original variables (i.e. signature peaks in the CHA-ZIF8 XRD spectrum) with the principal components determined by PCA. All principal components (PCs) were standardized to have mean at 0. Percent variance explains the percentage of total variance of the data explained by a particular principal component; PCs are listed in order of importance.

Principal components are interpreted by finding the most strongly correlated variables for each component. Strongly correlated variables have coefficients with large magnitudes (positive or negative). Correlations with magnitude greater than 0.5 were considered important, indicated in the table by the highlighted/boldfaced coefficients. The closer the coefficient is the 1, the more strongly the variable is correlated to the PC. Positive coefficients indicate that the variables (peak intensity or area) vary with the principal component, while negative coefficients imply an inverse variation.

Table S1. Principal component coefficients for peak intensity.

	PC 1	**PC 2**	**PC 3**	**PC 4**	**PC 5**	**PC 6**	**PC 7**	**PC 8**	**PC 9**
peak at 6.66	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1**
peak at 7.26	0.07	-0.06	-0.11	0.06	0.07	0.37	**0.91**	0.04	0
peak at 8.28	-0.11	0.26	**0.86**	-0.18	0.03	0.15	0.09	-0.33	0
peak at 9.26	**0.67**	**0.68**	-0.15	-0.22	0.10	-0.03	-0.01	0.05	0
peak at 10.64	**0.69**	**-0.67**	0.24	-0.15	-0.01	0.00	-0.05	-0.06	0
peak at 12.94	0.09	0.01	0.18	**0.58**	**0.78**	-0.07	-0.06	0.13	0
peak at 13.34	-0.07	0.00	0.31	-0.23	-0.05	-0.24	0.12	**0.88**	0
peak at 15.72	0.21	0.13	0.19	**0.69**	**-0.59**	-0.24	0.11	0.02	0
peak at 16.04	0.06	0.04	0.04	0.18	-0.15	**0.85**	-0.36	0.31	0
% variance	*70.48*	*19.54*	*5.36*	*2.52*	*1.04*	*0.54*	*0.36*	*0.15*	*0*

Table S2. Principal component coefficients for peak areas.

	PC 1	**PC 2**	**PC 3**	**PC 4**	**PC 5**	**PC 6**	**PC 7**	**PC 8**	**PC 9**
peak at 6.66	**0.60**	**-0.52**	-0.02	-0.59	0.09	0.03	-0.09	0.01	-0.03
peak at 7.26	0.10	0.01	-0.03	0.02	0.18	0.19	0.38	-0.24	**0.75**
peak at 8.28	**0.56**	**0.69**	-0.04	-0.08	-0.40	-0.02	-0.17	-0.05	0.08
peak at 9.26	-0.01	-0.16	**0.90**	0.04	-0.38	0.02	0.04	-0.11	0.06
peak at 10.64	0.36	-0.44	-0.25	**0.70**	-0.33	-0.08	-0.06	-0.06	0.04
peak at 12.94	0.21	0.09	0.02	0.12	0.13	0.49	**0.52**	-0.39	-0.51
peak at 13.34	0.14	0.03	0.01	-0.01	-0.12	-0.24	**0.67**	**0.68**	-0.04
peak at 15.72	0.08	0.02	0.11	0.18	0.13	**0.73**	-0.29	**0.56**	0.09
peak at 16.04	0.34	0.15	0.33	0.32	**0.70**	-0.36	-0.12	0.03	-0.05
% variance	*66.40*	*22.74*	*4.80*	*3.19*	*1.47*	*0.65*	*0.46*	*0.21*	*0.08*

Based on the variables identified by the first four principal components, which account for over 97% of the variance of both peak intensity and peak area with stacking fault rate (SFR), additional correlations of importance are shown in Figures S5 and S6.

Figure S6. Correlations of peak intensity to SFR, including standard deviation within each SFR.

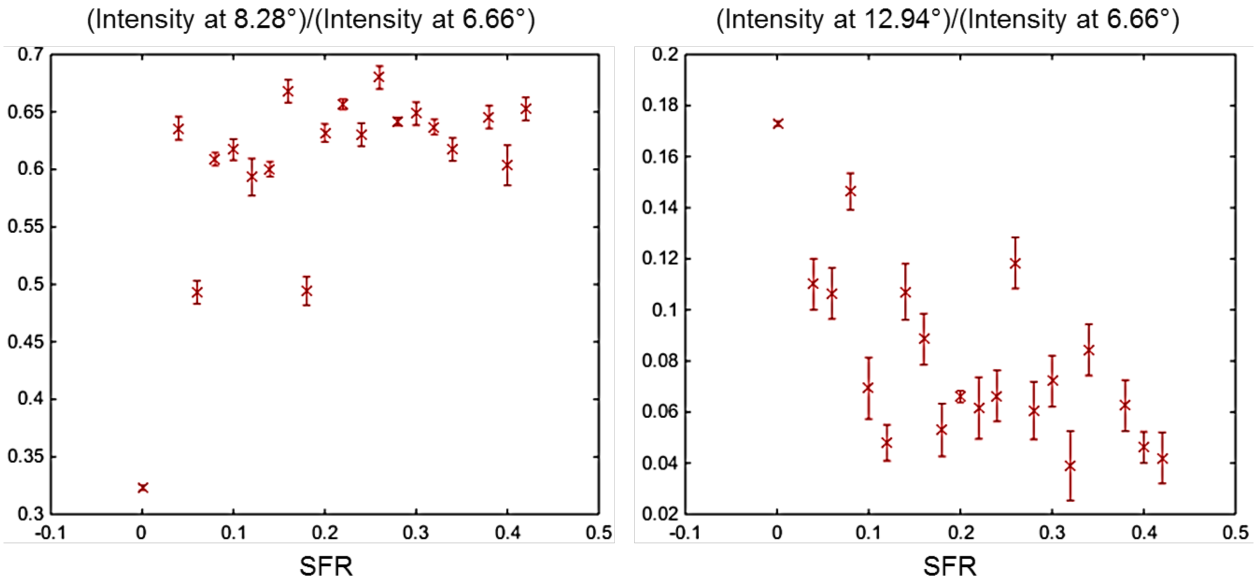
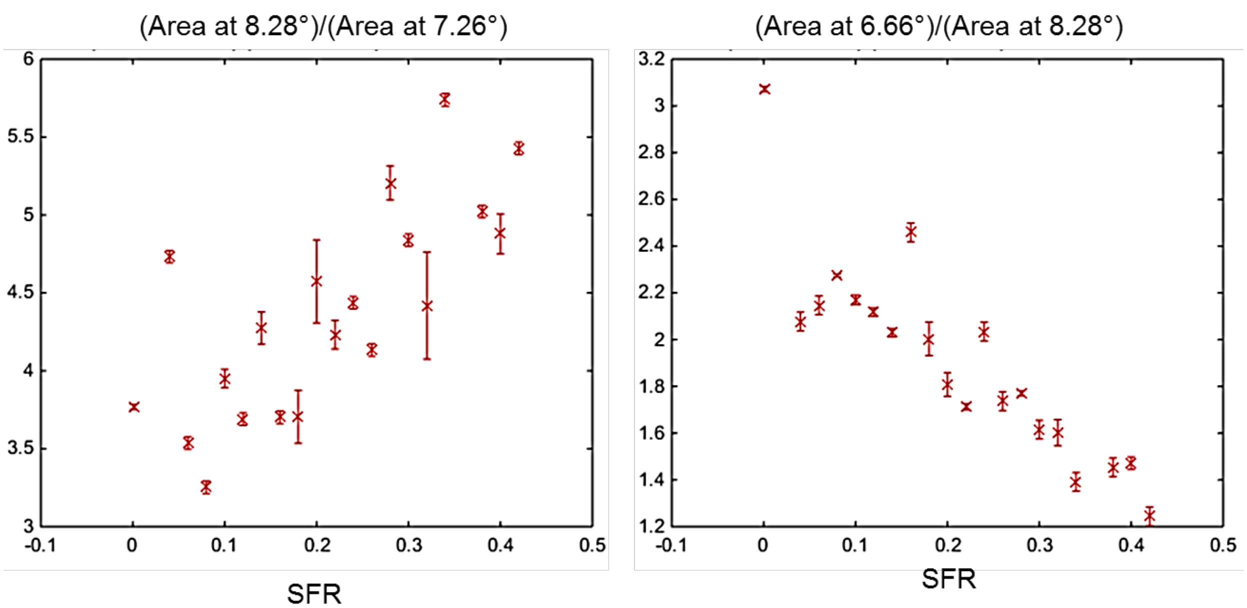


Figure S7. Correlations of peak areas to SFR, including standard deviation within each SFR.



Stacking fault effect on XRD of silica chabazite (CHA)

Figure S8. Comparison of silica chabazite (CHA) powder pattern and the peak broadening/splitting evident in an intergrowth structure (TS-C, reproduced from Li *et al.*[51]).