

Supplementary data:

Table S1: Crystallite size [nm] along (002), (100), (101), (102) and (110) crystallographic planes of reference ZnO and ZnO synthesized in the presence of different amino acids. The values in red represent crystallite size after mild thermal annealing. Red arrow indicates major decrease in crystallite size upon thermal annealing.

	Crystallite size [nm] (002) plane	Crystallite size [nm] (100) plane	Crystallite size [nm] (101) plane	Crystallite size [nm] (102) plane	Crystallite size [nm] (110) plane
ZnO	175.1 266.9	40.7 43.6	41.9 41.4	26.2 25.2	30.5 32.1
ZnO + aspartic acid	58.4 ▼ 47.2	34.3 36.6	34.5 34.9	22.2 23.3	27.8 28.7
ZnO + glutamic acid	222.1 ▼ 199.6	212.0 ▼ 184.2	102.3 130.1	84.7 107.1	126.9 ▼ 83.4
ZnO + cysteine	40.7 ▼ 26.2	23.6 16.0	17.4 23.3	11.2 13.7	16.6 13.5
ZnO + selenocystine	46.0 43.7	18.8 19.9	21.5 20.8	14.8 14.8	16.9 17.8
ZnO +serine	308.0 ▼ 90.2	193.7 ▼ 26.7	121.0 ▼ 94.2	155.8 ▼ 55.2	130.8 ▼ 46.7
ZnO + lysine	78.7 94.3	78.7 105.8	83.3 88.0	56.6 76.5	62.7 ▼ 43.1
ZnO + glycine	106.5 ▼ 62.3	31.3 34.5	33.0 34.2	22.0 22.9	27.5 28.0
ZnO + tyrosine	51.9 ▼ 40.2	24.8 25.5	25.0 25.3	16.0 16.4	20.0 19.9
ZnO + tryptophan	102.5 ▼ 48.6	30.0 33.7	30.5 31.8	18.3 20.0	25.0 26.2

Table S2: Microstrain fluctuations (μ -strain fluct.) along (002), (100), (101), (102) and (110) crystallographic planes of reference ZnO and ZnO synthesized in the presence of different amino acids. The numbers in red represent value after mild thermal annealing. Red arrow indicates major increase in microstrain fluctuations upon thermal annealing.

	μ -strain fluct. (002) plane	μ -strain fluct. (100) plane	μ -strain fluct. (101) plane	μ -strain fluct. (102) plane	μ -strain fluct. (110) plane
ZnO	3.02E-03 4.67E-04	1.11E-03 1.02E-03	7.62E-04 7.89E-04	7.75E-04 8.66E-04	7.79E-04 6.41E-04
ZnO + aspartic acid	2.70E-03 ▲ 3.30E-03	4.55E-03 4.52E-03	4.33E-03 4.64E-03	1.57E-03 1.29E-03	3.60E-03 4.19E-03
ZnO + glutamic acid	6.16E-04 ▲ 7.61E-03	6.37E-04 ▲ 9.27E-04	8.30E-04 9.42E-04	8.82E-04 8.91E-04	6.27E-04 9.43E-04
ZnO + cysteine	4.58E-03 ▲ 6.81E-03	1.82E-03 ▲ 3.00E-03	2.07E-03 ▲ 1.04E-02	2.21E-03 ▲ 1.51E-02	1.49E-03 1.48E-03
ZnO + selenocystine	3.26E-03 4.05E-03	1.16E-03 ▲ 9.23E-03	6.56E-03 5.91E-03	7.03E-04 9.31E-04	5.93E-03 5.98E-03
ZnO +serine	5.46E-04 ▲ 7.43E-03	8.21E-04 ▲ 1.31E-03	1.39E-03 ▲ 4.79E-03	1.31E-03 ▲ 7.80E-03	1.02E-03 ▲ 7.85E-03
ZnO + lysine	1.19E-03 ▲ 8.67E-03	1.19E-03 1.35E-03	1.20E-03 ▲ 7.94E-03	1.08E-03 ▲ 7.09E-03	1.21E-03 7.12E-04
ZnO + glycine	1.87E-03 ▲ 4.12E-03	4.38E-03 4.47E-03	4.57E-03 4.65E-03	1.36E-03 1.09E-03	3.60E-03 3.97E-03
ZnO + tyrosine	2.99E-03 ▲ 3.53E-03	6.88E-03 6.17E-03	5.48E-03 5.64E-03	3.21E-03 7.99E-03	4.29E-03 4.77E-03
ZnO + tryptophan	1.60E-03 ▲ 3.38E-03	4.68E-03 5.05E-03	4.43E-03 4.88E-03	1.80E-03 1.21E-03	3.60E-03 4.17E-03

Table S3: Change in crystallite size along (002) plane upon annealing (%), c-axis strain (%) and the change in band gap values before and after thermal annealing, of reference ZnO and ZnO synthesized in the presence of different amino acids.

Incorporated amino acid into ZnO	% change in crystallite size along (002) plane	% c-axis strain	ΔE_g [eV]
-	-52.4%	-	-
Aspartic acid	19.2%	0.097	0.02
Glutamic acid	10.1%	0.07	0.015
Cysteine	35.6%	0.203	0.12
Selenocysteine	5.0%	0.161	0.01
Serine	70.7%	0.031	0.03
Lysine	-19.8%	0.108	0.06
Glycine	41.5%	0.055	0.01
Tyrosine	22.5%	0.102	0.07
Tryptophan	52.6%	0.094	0.035