Supporting Information for:

Charge patching method for the calculation of Electronic Structure of Polypeptide

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We also applied the sum of neutral atoms to calculate the band gaps of these glycine polypeptides. The additional results are shown in the supporting information (SI). As one can see, our CPM is much better than the neutral atom sum results. As a matter of fact, the neutral atom sum is typically the starting point charge density in most DFT package (like the PWmat code). All of these calculations are based on PWmat code.

Table S1. The band gap of Gly-polypeptide in ribbon structures calculated by the CPM method, DFT with PBE calculations and sum of neutral atoms method(NONSCF calculation).

Gly-n-peptide	CPM method(eV)			DFT/PBE(eV)			NONSCF(eV)		
	HOMO	LUMO	GAP	HOMO	LUMO	GAP	HOMO	LUMO	GAP
6	-5.16	-1.60	3.56	-5.11	-1.48	3.63	-8.96	-3.53	5.43
7	-5.14	-1.57	3.57	-5.06	-1.44	3.62	-8.90	-3.47	5.43
8	-5.17	-1.50	3.66	-4.98	-1.45	3.53	-8.86	-3.41	5.45
9	-5.12	-1.61	3.50	-5.02	-1.42	3.60	-8.86	-3.45	5.41
10	-5.18	-1.53	3.65	-5.02	-1.37	3.66	-8.83	-3.39	5.44
11	-5.11	-1.64	3.48	-4.88	-1.51	3.37	-8.83	-3.43	5.40
12	-5.06	-1.73	3.33	-4.99	-1.44	3.55	-8.84	-3.47	5.37
13	-5.14	-1.64	3.50	-4.99	-1.39	3.60	-8.82	-3.42	5.41
14	-5.07	-1.75	3.32	-4.76	-1.64	3.12	-8.82	-3.46	5.36
15	-4.99	-1.84	3.15	-4.67	-1.74	2.92	-8.82	-3.50	5.32
16	-4.95	-1.93	3.02	-4.60	-1.83	2.78	-8.81	-3.54	5.28
17	-5.03	-1.85	3.19	-4.94	-1.45	3.49	-8.81	-3.49	5.32
18	-4.96	-1.95	3.01	-4.59	-1.81	2.78	-8.81	-3.53	5.28
19	-5.03	-1.87	3.15	-4.94	-1.44	3.49	-8.80	-3.48	5.32
20	-4.96	-1.97	3.00	-4.92	-1.48	3.44	-8.79	-3.52	5.27
21	-5.08	-1.87	3.21	-4.93	-1.44	3.49	-8.80	-3.48	5.32

22	-5.17	-1.78	3.39	-4.96	-1.39	3.57	-8.80	-3.43	5.37
23	-4.93	-1.83	3.09	-4.91	-1.51	3.40	-8.79	-3.55	5.24
24	-5.01	-1.75	3.25	-4.96	-1.46	3.50	-8.79	-3.51	5.28

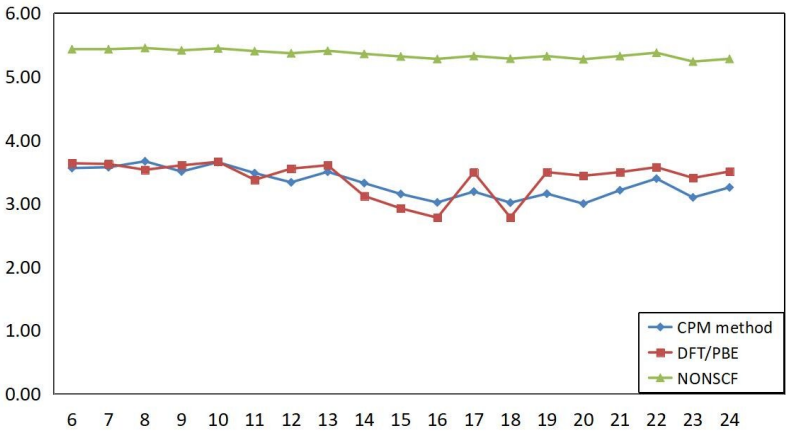

Figure S1. The band gap of ribbon structures calculated by the CPM, DFT with PBE calculations and sum of neutral atoms method(NONSCF calculation).

Table S2. The band gap of α-helix structures calculated by the CPM, DFT/PBE calculations and NONSCF calculation.

Gly-n-peptide	CPM method(eV)			DFT/PBE(eV)			NONSCF(eV)		
	HOMO	LUMO	GAP	HOMO	LUMO	GAP	HOMO	LUMO	GAP
6	-5.09	-2.17	2.92	-4.60	-1.55	3.05	-8.78	-3.18	5.60
7	-5.08	-2.08	3.00	-4.51	-1.48	3.03	-8.68	-3.09	5.60
8	-5.28	-2.17	3.12	-4.45	-1.49	2.96	-8.51	-3.00	5.51
9	-4.89	-2.28	2.61	-4.27	-1.70	2.57	-8.64	-3.11	5.53
10	-4.34	-2.54	1.80	-3.87	-1.94	1.93	-8.42	-3.07	5.34
11	-4.24	-2.34	1.91	-3.88	-1.68	2.20	-8.34	-2.97	5.37
12	-4.22	-2.72	1.50	-3.56	-2.15	1.41	-8.38	-3.11	5.27
13	-4.16	-2.60	1.56	-3.49	-2.08	1.40	-8.31	-3.04	5.28
14	-4.12	-2.53	1.60	-3.43	-2.13	1.30	-8.25	-2.98	5.27
15	-3.83	-3.00	0.83	-3.10	-2.54	0.56	-8.28	-3.11	5.17
16	-3.85	-2.86	0.98	-3.09	-2.49	0.61	-8.23	-3.04	5.18
17	-3.85	-2.70	1.15	-3.10	-2.37	0.73	-8.18	-2.98	5.20
18	-3.57	-3.15	0.41	-2.91	-2.66	0.25	-8.21	-3.10	5.10
19	-3.63	-3.25	0.38	-2.88	-2.61	0.26	-8.16	-3.05	5.12
20	-3.62	-3.21	0.42	-2.86	-2.59	0.28	-8.13	-2.99	5.14
21	-3.32	-3.31	0.01	-2.86	-2.69	0.16	-8.15	-3.11	5.04
22	-3.39	-3.37	0.02	-2.84	-2.55	0.29	-8.11	-3.06	5.05
23	-3.34	-3.10	0.24	-2.79	-2.57	0.22	-8.08	-3.00	5.07
24	-3.44	-3.11	0.33	-2.79	-2.54	0.24	-8.05	-2.94	5.11
25	-3.34	-3.10	0.24	-2.81	-2.60	0.21	-8.06	-3.07	4.99
26	-3.20	-3.16	0.04	-2.75	-2.59	0.16	-8.04	-3.01	5.03
27	-3.24	-3.08	0.17	-2.73	-2.57	0.17	-8.01	-2.96	5.05
two-18	-4.55	-2.42	2.13	-3.92	-1.79	2.13	-8.34	-2.97	5.36
two-19	-4.47	-2.46	2.01	-3.82	-1.76	2.06	-8.28	-2.93	5.35
two-20	-4.42	-2.21	2.21	-3.75	-1.73	2.02			
two-21	-4.36	-2.10	2.26	-3.82	-1.60	2.22			
two-22	-4.33	-2.24	2.09	-3.67	-1.61	2.06			
two-23	-4.23	-1.97	2.26	-3.61	-1.59	2.03			
two-24	-4.23	-1.84	2.39	-3.64	-1.47	2.16			
two-25	-4.23	-2.03	2.20	-3.63	-1.64	1.98			
two-26	-4.19	-1.89	2.30	-3.58	-1.58	2.00			
two-27	-4.14	-1.97	2.17	-3.45	-1.49	1.96			

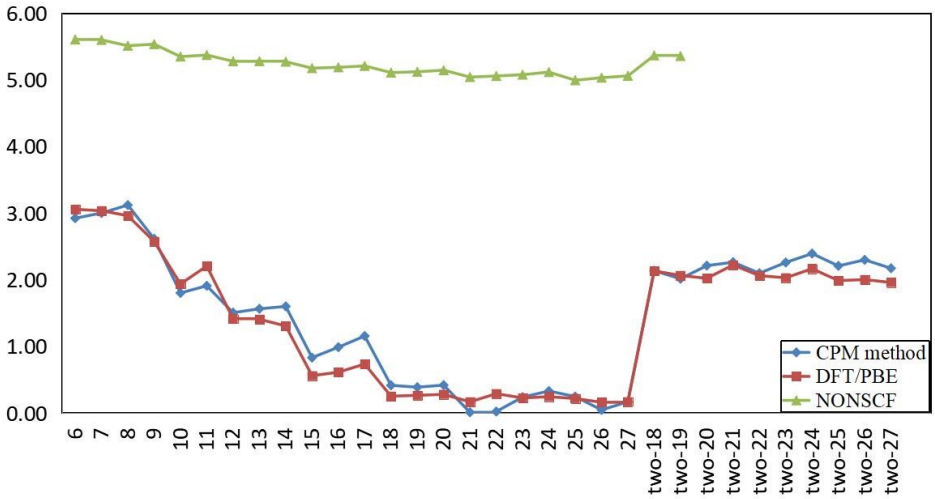

Figure S2. The band gap of α-helix structures calculated by the CPM, DFT/PBE and NONSCF calculation.

Table S3. The band gap of 3_{10}-helix structures calculated by the CPM, DFT/PBE calculations and NONSCF calculation.

Gly-n-polypeptide	CPM method(eV)			DFT/PBE(eV)			NONSCF(eV)		
	HOMO	LUMO	GAP	HOMO	LUMO	GAP	HOMO	LUMO	GAP
5	-5.46	-2.51	2.95	-4.74	-1.56	3.19	-8.88	-3.27	5.61
6	-5.43	-3.07	2.35	-4.53	-1.80	2.73	-8.87	-3.33	5.54
7	-5.39	-3.14	2.25	-4.38	-1.84	2.54	-8.79	-3.27	5.52
8	-5.26	-3.29	1.97	-4.19	-2.08	2.11	-8.79	-3.34	5.45
9	-5.50	-3.41	2.10	-3.92	-1.79	2.13	-8.68	-3.15	5.53
10	-5.28	-3.31	1.96	-4.05	-2.01	2.03	-8.67	-3.22	5.45
11	-5.13	-3.46	1.67	-3.84	-2.27	1.56	-8.67	-3.28	5.38
12	-4.99	-3.63	1.37	-3.64	-2.52	1.12	-8.67	-3.35	5.32
13	-5.23	-3.40	1.82	-3.89	-2.03	1.85	-8.59	-3.16	5.43
14	-5.05	-3.58	1.47	-3.64	-2.34	1.30	-8.59	-3.25	5.34
15	-5.11	-3.53	1.58	-3.69	-2.23	1.46	-8.56	-3.19	5.38
16	-4.96	-3.69	1.27	-3.45	-2.54	0.91	-8.56	-3.27	5.30
17	-5.01	-3.64	1.38	-3.57	-2.36	1.21	-8.54	-3.21	5.33
18	-4.85	-3.82	1.03	-3.31	-2.66	0.65	-8.54	-3.29	5.25
19	-4.92	-3.75	1.17	-3.52	-2.64	0.88	-8.52	-3.24	5.28
20	-5.01	-3.68	1.33	-3.38	-2.47	0.91	-8.50	-3.18	5.32
21	-5.12	-3.59	1.53	-3.51	-2.30	1.21	-8.49	-3.12	5.36
22	-5.27	-3.49	1.77	-3.67	-2.09	1.58	-8.48	-3.06	5.41
23	-5.03	-3.71	1.33	-3.41	-2.41	1.00	-8.48	-3.16	5.32
24	-5.18	-3.60	1.58	-3.54	-2.21	1.33	-8.47	-3.09	5.38
25	-4.94	-3.81	1.14	-3.45	-2.59	0.86	-8.46	-3.19	5.28
26	-5.07	-3.71	1.36	-3.38	-2.39	0.99	-8.47	-3.17	5.31

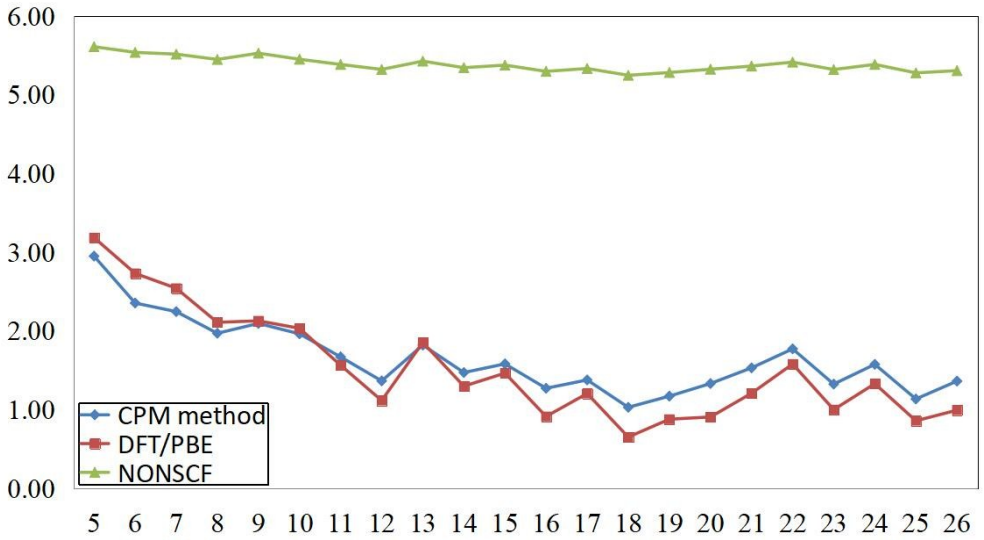

Figure S3. The band gap of 3_{10}-helix structures calculated by the CPM, DFT/PBE and NONSCF calculation.

Table S4. The band gap of β-strand structures calculated by the CPM, DFT/PBE calculations and NONSCF calculation.

Gly-n-polypeptide	CPM method(eV)			DFT/PBE(eV)			NONSCF(eV)		
	HOMO	LUMO	GAP	HOMO	LUMO	GAP	-9.18	-3.26	5.93
4	-6.64	-2.71	3.94	-5.18	-1.32	3.86	-9.15	-3.26	5.89
5	-6.67	-2.89	3.78	-5.13	-1.35	3.79	-9.12	-3.27	5.85
6	-6.71	-2.98	3.73	-5.05	-1.44	3.62	-9.06	-3.22	5.84
7	-6.79	-3.02	3.77	-5.00	-1.44	3.56	-9.05	-3.23	5.82
8	-6.81	-3.08	3.73	-5.20	-1.23	3.97	-9.05	-3.25	5.80
9	-6.82	-3.13	3.69	-5.20	-1.23	3.97	-9.01	-3.21	5.80
10	-6.92	-3.15	3.76	-5.15	-1.22	3.93	-9.00	-3.22	5.78
11	-6.93	-3.21	3.73	-5.16	-1.21	3.95	-9.00	-3.24	5.77
12	-6.93	-3.27	3.67	-5.17	-1.21	3.96	-9.00	-3.25	5.75
13	-6.94	-3.33	3.62	-5.18	-1.22	3.96	-8.97	-3.22	5.76
14	-7.05	-3.33	3.72	-5.14	-1.22	3.93	-9.00	-3.28	5.72
15	-7.06	-3.38	3.67	-5.21	-1.21	3.99	-8.97	-3.25	5.72
16	-7.04	-3.44	3.60	-5.08	-1.29	3.79	-8.96	-3.26	5.70
17	-7.18	-3.42	3.75	-5.14	-1.22	3.92	-9.18	-3.26	5.93

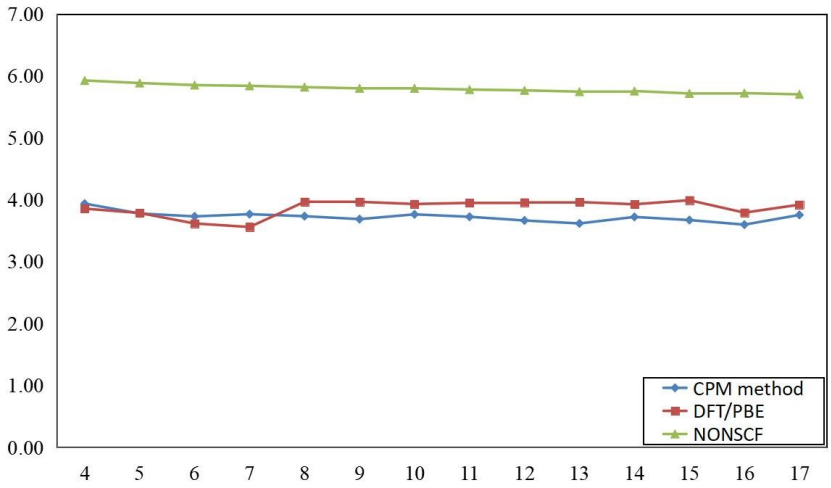

Figure S4. The band gap of β-strand structures calculated by the CPM, DFT/PBE and NONSCF calculation.