Supplementary Information

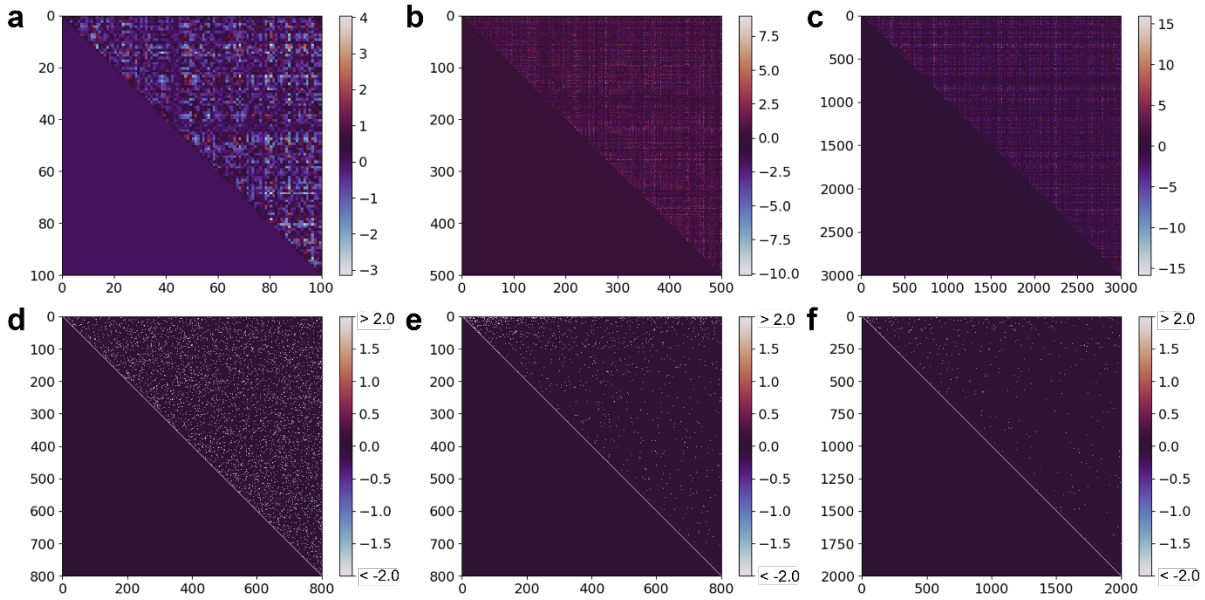

Fig. S1. Comparison of QUBO matrices for real-world optimization and Max-Cut problems. (**a**–**c**) QUBO matrices representing the optimization of planar multilayered structures (PMLs) with problem sizes of (**a**) 100, (**b**) 500, and (**c**) 3,000. The dense configurations of these matrices reflect the fully connected nature of interactions in material optimization problems. (**d**–**f**) QUBO matrices derived from Max-Cut problem instances in the G-set[S1]: (**d**) G5, (**e**) G15, and (**f**) G40. These matrices exhibit sparse configurations, with relatively few pairwise interactions compared to their maximum possible connections.

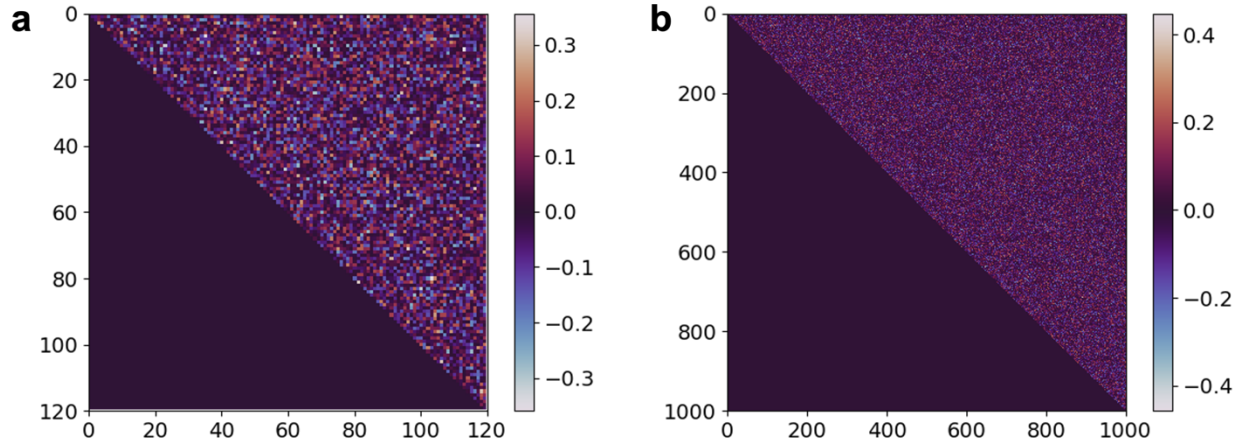

Fig. S2. Example QUBO matrices. The size of the given QUBO problems is (**a**) 120 and (**b**) 1,000 with a standard deviation of 0.1.

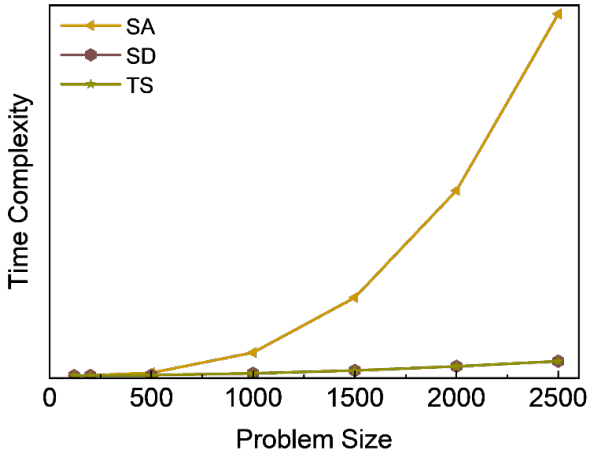

Fig. S3. Time complexity of simulated annealing (SA), steepest descent (SD), and tabu search (TS). This plot is from calculation results based on the theoretical time complexity (see 2-4-2. Computational Time in the main text), so it does not have metrics. The plot agrees well with the solving time plot depicted in Fig. 2b.

Table S1. Statistical properties of QUBO coefficients for real-world optimization problems. The table summarizes the average (avg) and standard deviation (std) of QUBO coefficients across different problem sizes (n). The average values of the coefficients are close to zero, and the standard deviation ranges from 0.2 to 2.

n	**50**	**100**	**200**	**500**	**1000**	**3000**	**5000**	**10000**
avg	0.0025	-0.0014	0.0003	-0.0004	0.0001	0.0016	0.0012	0.0008
std	0.2491	0.7440	0.8083	1.3319	1.5090	1.9519	2.0372	2.0706

Table S2. Density of Max-Cut problem instances. These instances feature sparse QUBO matrices with a density lower than 6%.

Instances	**# Nodes**	**# Edges**	**# Maximum Edges**	**Density (%)**
G5	800	19,176	319,600	6.0000
G10	800	19,176	319,600	6.0000
G15	800	4,661	319,600	1.4583
G20	800	4,672	319,600	1.4618
G30	2,000	19,900	1,999,000	0.9954
G40	2,000	11,766	1,999,000	0.5885
G50	3,000	6,000	4,498,500	0.1333
G55	5,000	12,498	12,497,500	0.1000
G60	7,000	17,148	24,496,500	0.0700
G70	10,000	9,999	49,995,000	0.0200

References

S1 Ye, Y. [online] Available: https://web.stanford.edu/~yyye/yyye/Gset/.