

Started GP relaxation phase 1.

param_gp =

-6.5452	-1.0714	-0.7804	-0.9521	1.1710	1.4812	1.2651	-0.7305	-0.3970	-0.7379
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Stopped GP relaxation phase 1: converged after 5645 iterations.

Accurate values: sumE_R = 4.08, maxnormF_R = 2.71, minnormF_R = 1.15, normFCI = 0

Started GP relaxation phase 2.

Warning: Function value at xnew not finite or a number

> In fminscg (line 214)

In gp_optim (line 121)

In GP_sNEB_orig (line 146)

In demo_tip4p (line 51)

param_gp =

-6.5452	-1.0714	-0.7804	-0.9521	1.1710	1.4812	1.2651	-0.7305	-0.3970	-0.7379
-3.3798	-1.2358	-0.5170	-1.1183	1.6866	1.0281	0.7179	-1.0887	-0.6093	-2.6840

Stopped GP relaxation phase 2: converged after 3027 iterations.

Accurate values: sumE_R = 11.7, maxnormF_R = 5.13, minnormF_R = 2.78, normFCI = 0

Started GP relaxation phase 3.

param_gp =

-6.5452	-1.0714	-0.7804	-0.9521	1.1710	1.4812	1.2651	-0.7305	-0.3970	-0.7379
-3.3798	-1.2358	-0.5170	-1.1183	1.6866	1.0281	0.7179	-1.0887	-0.6093	-2.6840
-1.7305	-0.5728	-0.4787	-2.8143	0.1357	0.9914	0.4281	-0.6082	-0.7315	-1.1841

Accurate values: sumE_R = 22.8, maxnormF_R = 15.1, minnormF_R = 4.86, normFCI = 0

Started GP relaxation phase 4.

param_gp =

-6.5452	-1.0714	-0.7804	-0.9521	1.1710	1.4812	1.2651	-0.7305	-0.3970	-0.7379
-3.3798	-1.2358	-0.5170	-1.1183	1.6866	1.0281	0.7179	-1.0887	-0.6093	-2.6840
-1.7305	-0.5728	-0.4787	-2.8143	0.1357	0.9914	0.4281	-0.6082	-0.7315	-1.1841
-0.5061	-1.1031	-1.1429	-2.3602	-0.3274	-0.8874	0.6235	-0.6459	-0.6293	-1.0519

Stopped GP relaxation phase 4: converged after 1331 iterations.

Accurate values: sumE_R = 28.1, maxnormF_R = 14.1, minnormF_R = 4.99, normFCI = 0

Started GP relaxation phase 5.

param_gp =

-6.5452	-1.0714	-0.7804	-0.9521	1.1710	1.4812	1.2651	-0.7305	-0.3970	-0.7379
-3.3798	-1.2358	-0.5170	-1.1183	1.6866	1.0281	0.7179	-1.0887	-0.6093	-2.6840

-1.7305	-0.5728	-0.4787	-2.8143	0.1357	0.9914	0.4281	-0.6082	-0.7315	-1.1841
-0.5061	-1.1031	-1.1429	-2.3602	-0.3274	-0.8874	0.6235	-0.6459	-0.6293	-1.0519
-0.0034	-0.7053	-0.8841	-2.0375	-0.2359	-0.6216	0.0225	-0.5460	-0.7575	-2.4423

Accurate values: sumE_R = 24.9, maxnormF_R = 11, minnormF_R = 2.91, normFCI = 0

Started GP relaxation phase 6.

param_gp =

-6.5452	-1.0714	-0.7804	-0.9521	1.1710	1.4812	1.2651	-0.7305	-0.3970	-0.7379
-3.3798	-1.2358	-0.5170	-1.1183	1.6866	1.0281	0.7179	-1.0887	-0.6093	-2.6840
-1.7305	-0.5728	-0.4787	-2.8143	0.1357	0.9914	0.4281	-0.6082	-0.7315	-1.1841
-0.5061	-1.1031	-1.1429	-2.3602	-0.3274	-0.8874	0.6235	-0.6459	-0.6293	-1.0519
-0.0034	-0.7053	-0.8841	-2.0375	-0.2359	-0.6216	0.0225	-0.5460	-0.7575	-2.4423
-0.1893	-1.2181	-1.2995	-1.5388	-0.3253	-0.5860	-0.4097	-1.0539	-1.1736	-2.4784

Accurate values: sumE_R = 32.4, maxnormF_R = 16.5, minnormF_R = 5.15, normFCI = 0

Started GP relaxation phase 7.

param_gp =

-6.5452	-1.0714	-0.7804	-0.9521	1.1710	1.4812	1.2651	-0.7305	-0.3970	-0.7379
-3.3798	-1.2358	-0.5170	-1.1183	1.6866	1.0281	0.7179	-1.0887	-0.6093	-2.6840
-1.7305	-0.5728	-0.4787	-2.8143	0.1357	0.9914	0.4281	-0.6082	-0.7315	-1.1841
-0.5061	-1.1031	-1.1429	-2.3602	-0.3274	-0.8874	0.6235	-0.6459	-0.6293	-1.0519
-0.0034	-0.7053	-0.8841	-2.0375	-0.2359	-0.6216	0.0225	-0.5460	-0.7575	-2.4423
-0.1893	-1.2181	-1.2995	-1.5388	-0.3253	-0.5860	-0.4097	-1.0539	-1.1736	-2.4784
0.0597	-0.9684	-1.4656	-1.2465	-0.1451	-0.2057	-0.4994	-2.8794	-0.9873	-1.4009

Accurate values: sumE_R = 30.1, maxnormF_R = 11.9, minnormF_R = 8.42, normFCI = 0

Started GP relaxation phase 8.

param_gp =

-6.5452	-1.0714	-0.7804	-0.9521	1.1710	1.4812	1.2651	-0.7305	-0.3970	-0.7379
-3.3798	-1.2358	-0.5170	-1.1183	1.6866	1.0281	0.7179	-1.0887	-0.6093	-2.6840
-1.7305	-0.5728	-0.4787	-2.8143	0.1357	0.9914	0.4281	-0.6082	-0.7315	-1.1841
-0.5061	-1.1031	-1.1429	-2.3602	-0.3274	-0.8874	0.6235	-0.6459	-0.6293	-1.0519
-0.0034	-0.7053	-0.8841	-2.0375	-0.2359	-0.6216	0.0225	-0.5460	-0.7575	-2.4423
-0.1893	-1.2181	-1.2995	-1.5388	-0.3253	-0.5860	-0.4097	-1.0539	-1.1736	-2.4784
0.0597	-0.9684	-1.4656	-1.2465	-0.1451	-0.2057	-0.4994	-2.8794	-0.9873	-1.4009
-0.1155	-1.8585	-1.4049	-1.4971	-0.4034	-0.3527	-0.4641	-2.2227	-1.6546	-1.2319

Stopped GP relaxation phase 8: converged after 2045 iterations.

Accurate values: sumE_R = 35, maxnormF_R = 17.7, minnormF_R = 6.59, normFCI = 0

Started GP relaxation phase 9.

param_gp =

-6.5452	-1.0714	-0.7804	-0.9521	1.1710	1.4812	1.2651	-0.7305	-0.3970	-0.7379
-3.3798	-1.2358	-0.5170	-1.1183	1.6866	1.0281	0.7179	-1.0887	-0.6093	-2.6840
-1.7305	-0.5728	-0.4787	-2.8143	0.1357	0.9914	0.4281	-0.6082	-0.7315	-1.1841
-0.5061	-1.1031	-1.1429	-2.3602	-0.3274	-0.8874	0.6235	-0.6459	-0.6293	-1.0519
-0.0034	-0.7053	-0.8841	-2.0375	-0.2359	-0.6216	0.0225	-0.5460	-0.7575	-2.4423
-0.1893	-1.2181	-1.2995	-1.5388	-0.3253	-0.5860	-0.4097	-1.0539	-1.1736	-2.4784
0.0597	-0.9684	-1.4656	-1.2465	-0.1451	-0.2057	-0.4994	-2.8794	-0.9873	-1.4009
-0.1155	-1.8585	-1.4049	-1.4971	-0.4034	-0.3527	-0.4641	-2.2227	-1.6546	-1.2319
-0.0650	-2.0917	-2.5189	-1.4814	-0.1182	-0.3510	-0.7311	-1.5387	-1.3084	-1.8831

Accurate values: sumE_R = 35.2, maxnormF_R = 17.5, minnormF_R = 6.3, normFCI = 0

Started GP relaxation phase 10.