Supplementary Materials

Searching new cocrystal structures of CL-20 and HMX *via* evolutionary algorithm and machine learning potential

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Supplementary Table 1. Comparison of enthalpy (E, unit: eV), density (ρ, unit: g/cm^3), and lattice constants of 1:2 HMX:CL-20 structures obtained by MLP and DFT optimization at zero pressure

ID	$method$	E	ρ	a(Å)	b(Å)	c(Å)	α(°)	β(°)	γ(°)
	DFT	-201.541	1.947	16.568	10.041	12.232	90.31	100.57	89.90
	MLP	-199.499	1.899	16.631	10.038	12.446	90.14	99.18	89.79
	DFT	-199.676	1.823	12.239	12.099	8.278	96.23	89.77	61.43
	MLP	-199.570	1.787	12.022	12.693	8.079	98.52	92.86	63.36
	DFT	-199.570	1.811	11.606	12.755	8.257	85.42	85.28	62.07
	MLP	-199.762	1.740	12.455	13.023	8.099	94.79	97.14	59.19
	DFT	-199.586	1.814	11.833	8.243	12.647	82.61	62.27	93.14
	MLP	-199.656	1.815	11.654	8.346	12.723	83.26	61.74	93.41
	DFT	-199.555	1.808	11.868	8.296	12.551	83.08	62.15	92.67
	MLP	-199.656	1.815	11.655	8.335	12.734	83.31	61.76	93.50
	DFT	-199.829	1.845	11.912	12.574	8.088	97.58	89.99	118.22
	MLP	-199.633	1.714	12.422	12.639	8.053	90.00	95.53	115.37
	DFT	-199.559	1.816	11.906	8.261	12.574	83.05	61.79	93.27
	MLP	-199.657	1.814	11.648	8.341	12.742	83.11	61.78	93.47
	DFT	-199.591	1.817	11.816	8.291	12.503	83.16	62.26	91.58
	MLP	-199.657	1.815	11.653	8.335	12.741	83.22	61.77	93.50
	DFT	-199.585	1.821	11.961	8.323	12.379	83.58	61.45	92.47
	MLP	-199.657	1.814	11.647	8.339	12.750	83.08	61.78	93.49
	DFT	-199.413	1.822	11.385	12.377	8.196	94.04	89.96	111.90
	MLP	-199.755	1.766	12.673	12.016	7.980	86.68	91.19	114.67
	DFT	-199.579	1.802	12.101	8.277	12.403	83.13	61.91	92.68

MLP	-199.657	1.815	11.650	8.342	12.736	83.18	61.76	93.44
DFT	-199.500	1.808	12.045	8.290	12.449	83.56	61.50	93.09
MLP	-199.657	1.814	11.648	8.341	12.740	83.15	61.77	93.46
DFT	-199.645	1.825	11.955	11.684	8.279	95.98	88.70	111.94
MLP	-199.592	1.780	13.168	10.875	8.064	90.90	88.44	108.66
DFT	-199.973	1.818	13.043	12.082	7.659	86.75	80.90	64.02
MLP	-200.192	1.831	13.821	12.079	7.075	91.30	85.62	64.76
DFT	-199.486	1.836	11.520	12.242	8.164	94.75	90.21	112.34
MLP	-199.766	1.768	12.687	11.979	7.980	86.90	91.19	114.61
DFT	-199.496	1.814	12.037	8.292	12.358	83.36	61.83	92.41
MLP	-199.656	1.815	11.659	8.336	12.724	83.40	61.74	93.48
DFT	-199.643	1.851	11.760	12.021	8.251	98.00	90.22	114.09
MLP	-199.539	1.782	12.503	12.440	8.089	102.10	91.23	116.40
DFT	-199.597	1.821	11.808	8.259	12.575	82.50	62.43	92.78
MLP	-199.657	1.814	11.645	8.338	12.752	83.05	61.79	93.50
DFT	-199.586	1.818	11.830	8.278	12.531	83.34	62.11	92.33
MLP	-199.657	1.814	11.648	8.341	12.743	83.12	61.78	93.47
DFT	-199.533	1.830	11.577	12.274	8.158	94.35	90.07	112.91
MLP	-199.765	1.768	12.686	11.983	7.980	86.87	91.19	114.62
DFT	-199.584	1.813	11.550	12.344	8.170	94.18	89.35	112.37
MLP	-199.578	1.772	13.278	10.881	8.025	89.34	88.81	108.56
DFT	-199.552	1.823	11.637	12.201	8.184	94.55	89.46	112.71
MLP	-199.607	1.764	13.366	10.891	8.002	89.31	88.77	108.56
DFT	-199.547	1.825	11.623	12.182	8.167	94.00	88.62	112.34
MLP	-199.612	1.763	13.365	10.900	8.003	89.46	88.71	108.65

DFT	-199.552	1.812	11.890	8.272	12.518	83.24	62.13	92.26
MLP	-199.657	1.815	11.654	8.334	12.739	83.26	61.76	93.51
DFT	-199.486	1.825	11.563	12.237	8.182	93.85	89.38	112.50
MLP	-199.707	1.735	13.529	11.055	7.966	88.11	88.19	109.39
DFT	-199.666	1.788	11.750	12.352	8.146	93.91	88.34	112.58
MLP	-199.680	1.737	12.621	12.376	7.996	90.43	82.75	115.06
DFT	-199.603	1.801	11.521	12.383	8.203	94.54	87.94	112.08
MLP	-199.595	1.769	13.325	10.873	8.023	89.67	88.62	108.70
DFT	-199.657	1.805	11.721	12.334	8.138	93.87	88.11	113.18
MLP	-199.589	1.771	13.300	10.875	8.028	89.62	88.66	108.67
DFT	-199.547	1.832	11.653	12.188	8.112	93.81	88.63	112.39
MLP	-199.710	1.736	13.511	11.067	7.976	88.50	88.04	109.68
DFT	-199.438	1.822	11.438	12.356	8.198	93.78	89.26	112.40
MLP	-199.596	1.768	13.332	10.876	8.016	89.53	88.68	108.63
DFT	-199.224	1.832	12.527	12.304	7.731	91.19	93.02	116.56
MLP	-200.003	1.811	13.116	12.497	7.612	96.70	85.04	119.74
DFT	-199.255	1.829	12.391	12.101	7.858	89.85	93.55	115.07
MLP	-199.996	1.822	13.061	12.374	7.582	96.26	85.76	118.66
DFT	-199.933	1.859	12.936	12.362	8.755	79.14	79.18	49.89
MLP	-200.185	1.843	14.279	13.121	7.710	90.95	97.58	47.84
DFT	-199.916	1.861	11.632	11.690	8.373	83.79	85.51	67.73
MLP	-199.895	1.806	12.759	10.719	8.423	89.01	97.11	70.94
DFT	-199.119	1.853	13.106	12.780	7.948	85.20	83.33	52.63
MLP	-199.559	1.804	13.996	13.691	7.568	88.27	86.13	48.24

DFT	-199.907	1.849	12.946	12.374	8.793	78.63	78.55	49.99
MLP	-200.155	1.841	14.192	13.030	7.757	90.01	96.48	48.24
DFT	-199.686	1.833	11.336	13.196	8.527	76.15	86.06	59.23
MLP	-199.925	1.855	10.383	14.461	8.366	72.07	83.06	61.44
DFT	-200.580	1.884	11.026	12.052	8.251	84.28	90.71	71.44
MLP	-199.896	1.850	11.179	12.262	8.105	84.08	93.03	72.91
DFT	-200.532	1.870	10.866	12.128	8.311	85.03	89.12	72.60
MLP	-199.896	1.850	11.181	12.260	8.107	84.07	93.05	72.95
DFT	-200.336	1.868	10.858	12.184	8.323	84.55	88.82	71.93
MLP	-199.699	1.854	10.867	11.827	8.732	80.91	82.06	71.13
DFT	-200.373	1.912	10.771	12.231	8.406	100.04	83.61	71.59
MLP	-199.006	1.866	12.059	12.346	7.959	95.00	80.07	65.32
DFT	-200.329	1.914	11.234	12.136	8.268	98.71	82.17	68.92
MLP	-199.029	1.858	12.028	12.360	8.016	95.25	80.39	65.12

Supplementary Table 2. Comparison of enthalpy (E, unit: eV), density (ρ, unit: g/cm^3), and lattice constants of 1:1 HMX:CL-20 cocrystal structures after optimization by MLP and DFT at zero pressure

ID	*method*	*E*	ρ	a(Å)	b(Å)	c(Å)	α(°)	β(°)	γ(°)
	DFT	-127.398	1.830	8.451	8.797	9.043	89.51	83.70	94.15
	MLP	-127.334	1.832	8.591	8.599	9.131	88.63	82.88	95.61
	DFT	-127.370	1.835	8.445	8.820	9.011	89.24	83.48	94.38
	MLP	-127.341	1.831	8.609	8.592	9.120	88.50	83.02	95.55
	DFT	-127.517	1.846	8.636	8.646	8.917	88.85	84.14	93.72
	MLP	-127.377	1.828	8.706	8.558	9.050	87.76	83.95	94.99
	DFT	-127.356	1.829	8.352	8.980	8.985	88.95	83.78	95.18
	MLP	-127.297	1.845	8.439	8.636	9.208	89.18	82.13	95.83
	DFT	-127.431	1.829	8.878	9.121	8.262	91.22	87.47	93.58
	MLP	-127.567	1.875	8.894	8.863	8.338	91.73	85.13	96.68
	DFT	-127.552	1.846	8.594	8.533	9.048	87.94	85.84	92.11
	MLP	-127.432	1.821	9.014	8.503	8.795	88.36	84.45	93.00
	DFT	-127.370	1.888	10.073	7.826	8.422	100.13	81.71	88.72
	MLP	-127.171	1.838	10.867	7.466	8.407	97.49	80.18	86.11
	DFT	-127.023	1.869	7.052	8.233	12.377	86.83	89.70	65.45
	MLP	-127.041	1.812	7.156	8.097	12.529	85.85	86.72	68.48
	DFT	-127.064	1.845	7.345	8.322	12.208	87.85	89.77	62.46
	MLP	-127.015	1.803	7.377	8.126	12.315	87.78	87.52	66.54
	DFT	-127.029	1.838	7.269	8.339	12.242	87.67	90.62	63.56
	MLP	-127.051	1.808	7.202	8.083	12.483	86.05	86.17	68.64
	DFT	-127.110	1.818	7.756	8.064	12.704	81.84	94.69	60.11

MLP	-127.473	1.822	7.734	8.226	12.275	82.27	94.39	61.22
DFT	-127.361	1.856	9.890	7.871	8.566	90.86	90.68	80.18
MLP	-127.821	1.812	9.556	7.714	9.367	82.14	94.86	81.72
DFT	-127.559	1.901	8.514	8.721	8.748	97.36	92.33	85.16
MLP	-127.725	1.887	8.315	8.732	9.049	98.76	92.01	84.43
DFT	-127.310	1.887	8.143	6.374	13.292	79.96	94.25	107.88
MLP	-127.371	1.842	8.264	6.519	13.264	79.42	95.01	109.46
DFT	-127.299	1.873	8.112	6.417	13.379	80.49	94.97	108.47
MLP	-127.365	1.839	8.256	6.543	13.259	79.45	95.12	109.60
DFT	-127.397	1.863	8.173	8.247	10.382	88.01	92.00	69.58
MLP	-127.542	1.839	7.911	8.085	10.868	87.19	92.33	73.08
DFT	-127.282	1.900	8.470	6.351	13.375	79.75	86.33	65.08
MLP	-127.259	1.822	8.330	7.204	13.494	79.36	86.58	57.35
DFT	-127.265	1.850	8.368	10.077	7.937	93.75	99.21	90.49
MLP	-127.326	1.871	8.295	10.445	7.906	93.41	107.54	87.54
DFT	-127.401	1.885	8.780	8.532	8.815	91.51	98.30	82.10
MLP	-127.774	1.892	8.348	9.611	8.177	91.88	96.07	81.12
DFT	-127.242	1.850	8.454	10.032	7.883	92.60	99.13	90.12
MLP	-127.332	1.874	8.300	10.437	7.883	93.25	107.27	87.40
DFT	-127.290	1.847	8.372	10.109	7.915	94.04	98.72	90.77
MLP	-127.336	1.867	8.316	10.447	7.894	93.29	107.42	87.67
DFT	-127.265	1.848	8.415	10.078	7.904	93.50	99.38	90.09
MLP	-127.334	1.871	8.306	10.449	7.890	93.35	107.49	87.60
DFT	-127.248	1.845	8.444	10.129	7.850	92.86	99.69	90.05
MLP	-127.329	1.874	8.298	10.434	7.885	93.23	107.24	87.37

DFT	-127.257	1.849	8.499	10.058	7.822	92.37	99.10	89.89
MLP	-127.335	1.869	8.312	10.450	7.892	93.33	107.48	87.67
DFT	-127.684	1.869	9.077	8.337	8.909	100.70	82.30	97.48
MLP	-127.541	1.838	9.088	8.533	8.814	101.30	83.66	96.33
DFT	-127.367	1.883	8.225	8.390	9.571	82.85	96.75	96.38
MLP	-127.540	1.840	8.574	8.763	9.091	83.73	96.46	101.28
DFT	-127.396	1.884	8.295	8.319	9.570	82.88	96.92	96.56
MLP	-127.538	1.841	8.631	8.695	9.095	83.82	96.60	101.23
DFT	-127.694	1.865	9.004	8.320	9.011	100.80	82.05	96.71
MLP	-127.541	1.839	9.088	8.537	8.808	101.30	83.67	96.34
DFT	-127.279	1.848	8.359	10.136	7.902	93.29	98.97	91.08
MLP	-127.335	1.867	8.314	10.450	7.897	93.34	107.50	87.70
DFT	-127.413	1.862	8.360	8.835	8.976	89.82	81.13	90.42
MLP	-127.362	1.812	8.134	8.703	9.702	91.43	82.52	98.69
DFT	-127.386	1.872	8.227	8.419	9.577	83.00	96.31	96.11
MLP	-127.539	1.840	8.599	8.732	9.092	83.77	96.53	101.26
DFT	-127.394	1.881	8.259	8.316	9.612	82.82	96.11	95.93
MLP	-127.539	1.840	8.603	8.727	9.093	83.78	96.54	101.25
DFT	-127.447	1.923	8.144	8.491	9.343	98.31	90.83	82.73
MLP	-127.264	1.921	8.113	8.338	9.524	97.91	90.94	84.15
DFT	-127.460	1.914	8.074	8.502	9.455	98.48	90.97	83.06
MLP	-127.295	1.907	7.934	8.318	9.877	100.13	92.69	85.73
DFT	-127.511	1.918	8.068	8.424	9.525	98.40	90.70	82.99
MLP	-127.367	1.903	8.283	8.339	9.455	99.53	92.43	84.61

DFT	-127.475	1.916	8.070	8.479	9.474	98.17	90.54	82.75
MLP	-127.367	1.903	8.283	8.336	9.460	99.54	92.42	84.61
DFT	-127.502	1.918	8.243	8.643	9.064	97.81	90.76	83.75
MLP	-126.950	1.935	8.349	8.556	8.932	96.71	90.28	83.90
DFT	-127.504	1.923	8.255	8.678	9.002	98.10	90.62	83.43
MLP	-126.950	1.935	8.349	8.556	8.934	96.72	90.28	83.90
DFT	-127.499	1.925	8.205	8.666	9.055	98.10	90.51	83.40
MLP	-126.950	1.936	8.351	8.555	8.931	96.69	90.28	83.90
DFT	-127.451	1.925	8.119	8.420	9.443	98.30	90.69	82.56
MLP	-127.779	1.898	8.177	8.400	9.535	98.76	91.82	83.03
DFT	-127.457	1.918	8.153	8.548	9.259	98.18	90.33	84.35
MLP	-126.950	1.935	8.350	8.555	8.932	96.70	90.28	83.90
DFT	-127.466	1.924	8.223	8.731	8.969	97.28	89.21	83.11
MLP	-127.795	1.897	8.153	8.382	9.589	98.98	91.70	83.37
DFT	-127.545	1.914	8.051	9.604	8.403	81.04	83.05	89.45
MLP	-127.776	1.897	8.147	9.660	8.328	80.92	83.49	88.29
DFT	-127.498	1.903	8.877	8.353	8.705	84.62	86.35	91.67
MLP	-127.780	1.906	9.001	8.266	8.662	83.40	88.43	87.21
DFT	-127.354	1.879	11.690	8.364	6.709	91.57	96.94	85.42
MLP	-127.185	1.867	11.598	8.025	7.247	89.54	103.03	84.03