processes

Supplementary Material

Insights on the Separation of Kraft Lignin from Betaine-Based Eutectic Solvents: A Liquid-Liquid Equilibrium and Partitioning Study

Fernanda Sossai Altoé, Dulce Maria Santos, Sérgio M. Vilas-Boas * and Mariana Conceição da Costa *

Department of Process and Product Design (DDPP), School of Chemical Engineering (FEQ), University of Campinas (UNICAMP), Av. Albert Einstein, 500, Campinas, São Paulo, 13083- 852, Brazil;
* Correspondence: svboas@unicamp.br (S.M.V.-B.); mcdcosta@unicamp.br (M.C.d.C.)

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Calibration Curve

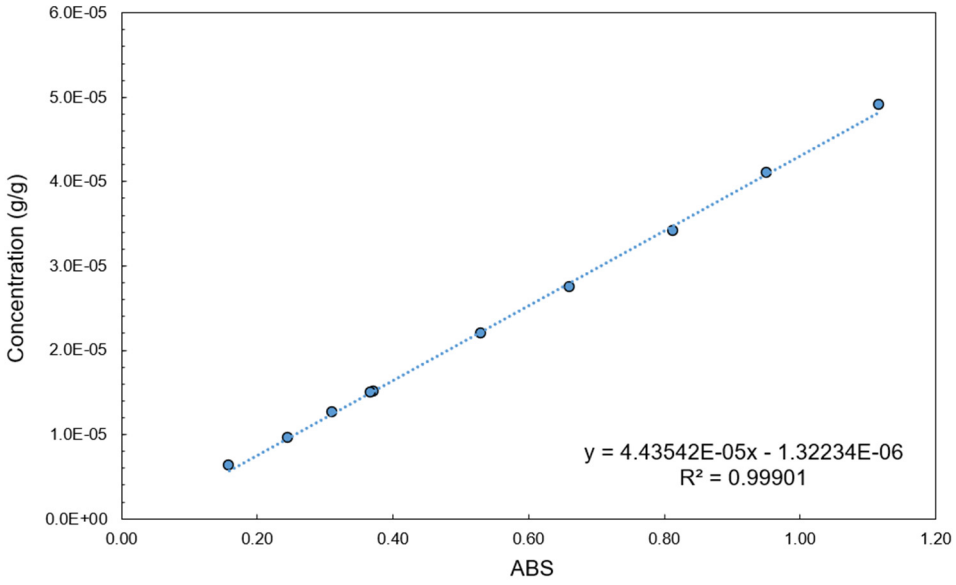


Figure S1. Calibration curve of the UV-Vis spectrophotometric analysis of Kraft lignin. The plot shows the Kraft lignin concentration in dimethyl sulfoxide (g/g) (y-axis) as a function of the absorbance at 280 nm (x-axis). The line represents the linear regression used to determine the lignin concentrations in the experiments.

Binodal Curves

Table S1. Experimental mass fraction (w) data for the binodal curve of {1-butanol (1) + Water (2) + BET:U (3)} at 298.15 K and 95.0 kPa.

1-Butanol (1) + Water (2) + BET:U (3)								
w_1	w_2	w_3	w_1	w_2	w_3	w_1	w_2	w_3
0.857	0.132	0.011	0.450	0.359	0.191	0.068	0.732	0.200
0.775	0.172	0.053	0.404	0.386	0.210	0.067	0.754	0.179
0.754	0.182	0.064	0.369	0.407	0.224	0.065	0.787	0.148
0.704	0.210	0.086	0.333	0.429	0.238	0.063	0.801	0.136
0.672	0.229	0.099	0.291	0.455	0.254	0.066	0.820	0.114
0.629	0.255	0.116	0.259	0.476	0.265	0.064	0.833	0.103
0.592	0.276	0.132	0.214	0.501	0.285	0.070	0.856	0.074
0.570	0.289	0.132	0.181	0.521	0.298	0.075	0.877	0.048
0.542	0.307	0.151	0.064	0.715	0.221	0.083	0.917	0.000
0.498	0.329	0.173						

Table S2. Experimental mass fraction (w) data for the binodal curve of {ethyl acetate (1) + water (2) + BET:U (3)} at 298.15 K and 95.0 kPa.

Ethyl Acetate (1) + Water (2) + BET:U (3)								
w_1	w_2	w_3	w_1	w_2	w_3	w_1	w_2	w_3
0958	0.042	0.000	0.640	0.283	0.077	0.303	0.543	0.154
0.931	0.059	0.010	0.602	0.313	0.085	0.270	0.567	0.163
0.885	0.094	0.021	0.555	0.348	0.097	0.237	0.594	0.169
0.850	0.120	0.030	0.518	0.377	0.105	0.072	0.845	0.083
0.827	0.138	0.035	0.481	0.404	0.115	0.073	0.856	0.071
0.804	0.158	0.038	0.443	0.434	0.123	0.074	0.873	0.053
0.775	0.180	0.045	0.419	0.451	0.130	0.078	0.890	0.032
0.746	0.202	0.052	0.399	0.469	0.132	0.078	0.896	0.026
0.708	0.232	0.060	0.369	0.491	0.140	0.096	0.904	0.000
0.673	0.258	0.069	0.336	0.517	0.147			

Table S3. Experimental mass fraction (w) data for the binodal curve of {1-butanol (1) + water (2) + BET:EG (3)} at 298.15 K and 95.0 kPa.

1-Butanol (1) + Water (2) + BET:EG (3)								
w_1	w_2	w_3	w_1	w_2	w_3	w_1	w_2	w_3
0.836	0.118	0.046	0.432	0.300	0.268	0.071	0.731	0.198
0.798	0.134	0.068	0.406	0.312	0.282	0.072	0.748	0.181
0.772	0.145	0.083	0.379	0.325	0.296	0.073	0.767	0.160
0.742	0.158	0.100	0.341	0.344	0.315	0.074	0.786	0.140
0.716	0.170	0.114	0.296	0.366	0.338	0.077	0.803	0.120
0.691	0.181	0.128	0.271	0.375	0.354	0.076	0.822	0.102
0.645	0.201	0.154	0.062	0.635	0.303	0.076	0.840	0.084
0.591	0.226	0.183	0.066	0.655	0.279	0.078	0.856	0.066
0.564	0.239	0.197	0.067	0.674	0.259	0.077	0.872	0.051
0.537	0.251	0.212	0.070	0.695	0.235	0.082	0.901	0.017
0.512	0.263	0.225	0.070	0.711	0.219	0.083	0.917	0.000
0.488	0.274	0.238						

Table S4. Experimental mass fraction (w) data for the binodal curve {ethyl acetate (1) + water (2) + BET:EG (3)} at 298.15 K and 95.0 kPa.

Ethyl Acetate (1) + Water (2) + BET:EG (3)								
w_1	w_2	w_3	w_1	w_2	w_3	w_1	w_2	w_3
0.958	0.042	0.000	0.623	0.270	0.107	0.356	0.460	0.184
0.922	0.059	0.019	0.588	0.295	0.117	0.328	0.480	0.192
0.878	0.092	0.030	0.557	0.317	0.126	0.288	0.508	0.204
0.851	0.111	0.038	0.526	0.339	0.135	0.247	0.537	0.216
0.822	0.133	0.045	0.497	0.358	0.145	0.070	0.823	0.107
0.792	0.153	0.055	0.471	0.376	0.153	0.071	0.844	0.085
0.758	0.176	0.066	0.449	0.391	0.160	0.078	0.875	0.047
0.723	0.201	0.076	0.416	0.414	0.170	0.082	0.894	0.024
0.692	0.222	0.086	0.384	0.439	0.177	0.096	0.904	0.000
0.658	0.246	0.096						

Table S5. Experimental mass fraction (w) data for the binodal curve of {1-butanol (1) + water (2) + BET:PROP (3)} at 298.15 K and 95.0 kPa.

1-Butanol (1) + Water (2) + BET:PROP (3)								
w_1	w_2	w_3	w_1	w_2	w_3	w_1	w_2	w_3
0.083	0.917	0.000	0.690	0.169	0.141	0.278	0.389	0.333
0.077	0.895	0.028	0.735	0.155	0.110	0.318	0.351	0.331
0.078	0.860	0.062	0.756	0.145	0.099	0.341	0.330	0.329
0.079	0.817	0.104	0.797	0.130	0.073	0.366	0.309	0.325
0.080	0.775	0.145	0.835	0.120	0.045	0.406	0.285	0.309
0.085	0.736	0.179	0.131	0.567	0.302	0.443	0.268	0.289
0.091	0.693	0.216	0.147	0.542	0.311	0.485	0.249	0.266
0.101	0.647	0.252	0.166	0.513	0.321	0.509	0.241	0.250
0.112	0.612	0.276	0.190	0.482	0.328	0.538	0.228	0.234
0.620	0.196	0.184	0.210	0.460	0.330	0.567	0.216	0.217
0.657	0.181	0.162	0.242	0.424	0.334			

Table S6. Experimental mass fraction (w) data for the binodal curve of {ethyl acetate (1) + water (2) + BET:PROP (3)} at 298.15 K and 95.0 kPa.

Ethyl Acetate (1) + Water (2) + BET:PROP (3)								
w_1	w_2	w_3	w_1	w_2	w_3	w_1	w_2	w_3
0.096	0.904	0.000	0.408	0.419	0.173	0.646	0.253	0.101
0.088	0.884	0.028	0.439	0.398	0.163	0.673	0.234	0.093
0.086	0.872	0.042	0.473	0.377	0.150	0.697	0.217	0.085
0.083	0.843	0.074	0.958	0.042	0.000	0.721	0.200	0.079
0.080	0.814	0.106	0.499	0.356	0.145	0.746	0.183	0.071
0.269	0.517	0.214	0.534	0.332	0.134	0.773	0.164	0.063
0.306	0.491	0.203	0.556	0.316	0.128	0.809	0.138	0.053
0.345	0.463	0.192	0.592	0.291	0.117	0.842	0.115	0.043
0.375	0.442	0.183	0.619	0.272	0.109	0.889	0.082	0.029

Table S7. Experimental mass fraction (w) data for the binodal curve of {1-butanol (1) + water (2) + BET:BUT (3)} at 298.15 K and 95.0 kPa.

1-Butanol (1) + Water (2) + BET:BUT (3)								
w_1	w_2	w_3	w_1	w_2	w_3	w_1	w_2	w_3
0.083	0.917	0.000	0.291	0.522	0.187	0.454	0.354	0.192
0.078	0.888	0.034	0.301	0.510	0.189	0.476	0.332	0.192
0.080	0.848	0.072	0.322	0.488	0.190	0.498	0.311	0.191
0.089	0.809	0.102	0.189	0.632	0.179	0.520	0.290	0.190
0.106	0.762	0.132	0.357	0.448	0.195	0.777	0.179	0.044
0.123	0.726	0.151	0.372	0.438	0.190	0.806	0.194	0.000
0.232	0.583	0.185	0.406	0.402	0.192	0.792	0.182	0.026
0.242	0.563	0.195	0.430	0.378	0.192	0.264	0.547	0.189
0.217	0.599	0.184						

Table S8. Experimental mass fraction (w) data for the binodal curve of {ethyl acetate (1) + water (2) + BET:BUT (3)} at 298.15 K and 95.0 kPa.

Ethyl Acetate (1) + Water (2) + BET:BUT (3)								
w_1	w_2	w_3	w_1	w_2	w_3	w_1	w_2	w_3
0.096	0.904	0.000	0.627	0.270	0.103	0.489	0.371	0.140
0.096	0.835	0.069	0.602	0.290	0.108	0.467	0.386	0.147
0.847	0.117	0.036	0.580	0.306	0.114	0.439	0.407	0.154
0.850	0.111	0.039	0.556	0.324	0.120	0.414	0.427	0.159
0.830	0.125	0.045	0.534	0.341	0.125	0.394	0.441	0.165
0.801	0.145	0.054	0.958	0.042	0.000	0.370	0.460	0.170
0.767	0.169	0.064	0.931	0.057	0.012	0.352	0.472	0.176
0.739	0.188	0.073	0.881	0.091	0.028	0.332	0.487	0.181
0.713	0.208	0.079	0.559	0.325	0.116	0.310	0.504	0.186
0.679	0.232	0.089	0.532	0.341	0.127	0.099	0.873	0.028
0.653	0.251	0.096	0.507	0.359	0.134	0.098	0.849	0.053

Table S9. Et(30) parameters for alcohol HBDs studied in this work.

HBD	Et(30) [kcal.mol^{-1}]	Reference
ethylene glycol	53.8	[1]
1,3-propanediol	54.9	[1]
1,4-butanediol	52.6	[1]

Kraft Lignin Partitioning

Table S10. Global compositions (w), phase densities (d_{Top} and d_{Bottom}), and Kraft lignin partition coefficients (K_{Lignin}) for the {1-butanol (1) + water (2) + BET:U (3)} system.

Global Composition	w_1	w_2	w_3	d_{Top} (g/cm^3)	d_{Bottom} (g/cm^3)	K_{Lignin}
1	0.430	0.547	0.022	0.8436	0.9943	2.9
2	0.446	0.490	0.064	0.8422	1.0071	1.6
3	0.408	0.493	0.098	0.8413	1.0207	1.2
4	0.388	0.487	0.125	0.8410	1.0269	1.1
5	0.370	0.467	0.163	0.8396	1.0396	0.9

Table S11. Global compositions (w), phase densities (d_{Top} and d_{Bottom}), and Kraft lignin partition coefficients (K_{Lignin}) for the {ethyl acetate (1) + water (2) + BET:U (3)} system.

Global Composition	w_1	w_2	w_3	d_{Top} (g/cm³)	d_{Bottom} (g/cm³)	K_{Lignin}
1	0.491	0.496	0.013	0.8992	0.9994	4.6
2	0.470	0.498	0.033	0.8993	1.0076	3.0
3	0.460	0.486	0.054	0.8992	1.0153	1.8
4	0.438	0.481	0.081	0.8991	1.0220	1.5
5	0.410	0.480	0.110	0.8992	1.0310	1.2

Table S12. Global compositions (w), phase densities (d_{Top} and d_{Bottom}), and Kraft lignin partition coefficients (K_{Lignin}) for the {1-butanol (1) + water (2) + BET:EG (3)} system.

Global Composition	w_1	w_2	w_3	d_{Top} (g/cm³)	d_{Bottom} (g/cm³)	K_{Lignin}
1	0.450	0.499	0.052	0.8459	1.0002	22.3
2	0.420	0.478	0.102	0.8482	1.0118	11.6
3	0.401	0.446	0.153	0.8507	1.0227	6.5
4	0.371	0.426	0.204	0.8556	1.0318	4.7
5	0.350	0.396	0.254	0.8600	1.0412	2.9

Table S13. Global compositions (w), phase densities (d_{Top} and d_{Bottom}), and Kraft lignin partition coefficients (K_{Lignin}) for the {ethyl acetate (1) + water (2) + BET:EG (3)} system.

Global Composition	w_1	w_2	w_3	d_{Top} (g/cm³)	d_{Bottom} (g/cm³)	K_{Lignin}
1	0.490	0.499	0.011	0.8996	0.9973	23.8
2	0.468	0.498	0.034	0.8992	1.0046	13.1
3	0.465	0.483	0.052	0.8992	1.0091	11.3
4	0.459	0.469	0.072	0.8992	1.0146	10.2
5	0.450	0.447	0.103	0.8993	1.0222	7.2

Table S14. Global compositions (w), phase densities (d_{Top} and d_{Bottom}), and Kraft lignin partition coefficients (K_{Lignin}) for the {1-butanol (1) + water (2) + BET:PROP (3)} system.

Global Composition	w_1	w_2	w_3	d_{Top} (g/cm³)	d_{Bottom} (g/cm³)	K_{Lignin}
1	0.450	0.498	0.052	0.8511	0.9946	60.4
2	0.420	0.478	0.102	0.8558	1.0012	30.1
3	0.401	0.446	0.153	0.8659	1.0083	8.8
4	0.370	0.427	0.203	0.8768	1.0130	4.8
5	0.350	0.396	0.254	0.8898	1.0162	2.9

Table S15. Global compositions (w), phase densities (d_{Top} and d_{Bottom}), and Kraft lignin partition coefficients (K_{Lignin}) for the {ethyl acetate (1) + water (2) + BET:PROP (3)} system.

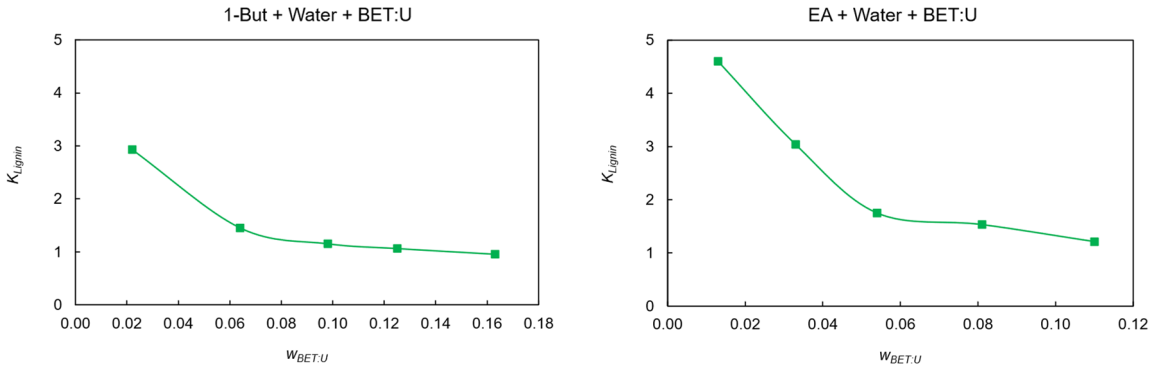
Global Composition	w_1	w_2	w_3	d_{Top} (g/cm³)	d_{Bottom} (g/cm³)	K_{Lignin}
1	0.499	0.490	0.011	0.8998	0.9984	15.3
2	0.469	0.500	0.031	0.8996	1.0054	13.6
3	0.460	0.489	0.051	0.9010	1.0048	11.1
4	0.431	0.497	0.072	0.9004	1.0076	7.9
5	0.399	0.500	0.100	0.9007	1.0115	8.5

Table S16. Global compositions (w), phase densities (dTop and d_{Bottom}), and Kraft lignin partition coefficients (K_{Lignin}) for the {1-butanol (1) + water (2) + BET:BUT (3)} system.

Global Composition	w_1	w_2	w_3	d_{Top} (g/cm³)	d_{Bottom} (g/cm³)	K_{Lignin}
1	0.472	0.463	0.065	0.8605	0.9907	456.5
2	0.440	0.477	0.083	0.8662	0.9912	196.8
3	0.419	0.480	0.101	0.8721	0.9913	172.4
4	0.440	0.447	0.113	0.8763	0.9924	98.9
5	0.399	0.468	0.133	0.8850	0.9904	89.8

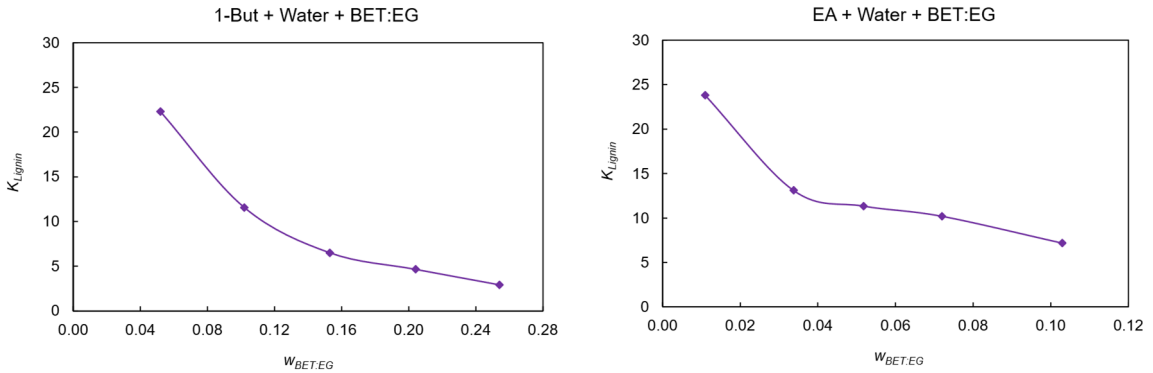
Table S17. Global compositions (w), phase densities (dTop and d_{Bottom}), and Kraft lignin partition coefficients (K_{Lignin}) for the {ethyl acetate (1) + water (2) + BET:BUT (3)} system.

Global Composition	w_1	w_2	w_3	d_{Top} (g/cm³)	d_{Bottom} (g/cm³)	K_{Lignin}
1	0.468	0.482	0.050	0.9016	1.0025	24.7
2	0.470	0.465	0.066	0.9012	1.0011	28.9
3	0.465	0.455	0.080	0.9018	1.0037	17.0
4	0.469	0.430	0.100	0.9023	1.0056	4.8
5	0.437	0.433	0.130	0.9024	1.0074	4.5



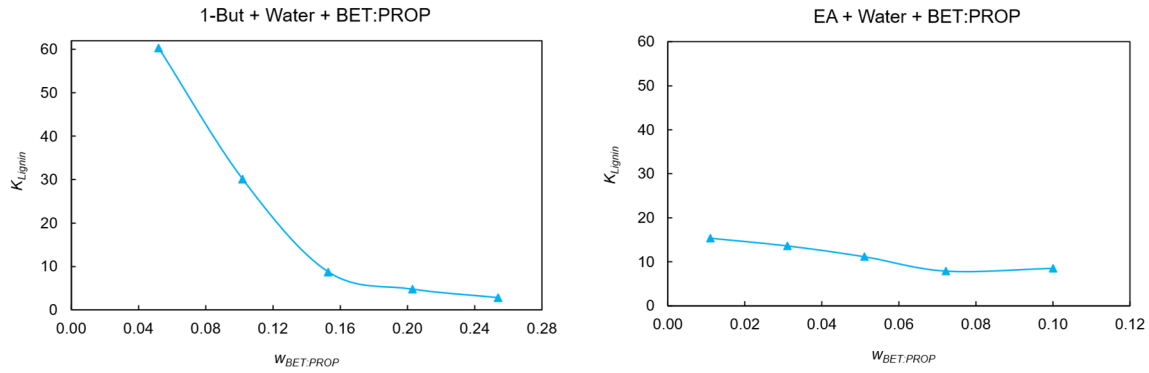
(**a**) (**b**)

Figure S2. Kraft lignin partition coefficient as a function of the overall mass fraction of the BET:U eutectic solvent for systems containing (**a**) 1-butanol and (**b**) ethyl acetate.



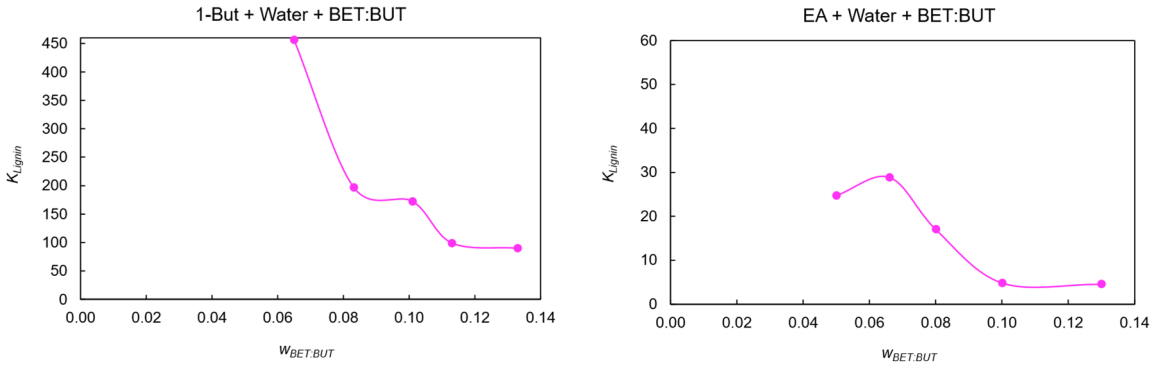
(**a**) (**b**)

Figure S3. Kraft lignin partition coefficient as a function of the overall mass fraction of the BET:EG eutectic solvent for systems containing (**a**) 1-butanol and (**b**) ethyl acetate.



(**a**) (**b**)

Figure S4. Kraft lignin partition coefficient as a function of the overall mass fraction of the BET:PROP eutectic solvent for systems containing (**a**) 1-butanol and (**b**) ethyl acetate.



(**a**) (**b**)

Figure S5. Kraft lignin partition coefficient as a function of the overall mass fraction of the BET:BUT eutectic solvent for systems containing (**a**) 1-butanol and (**b**) ethyl acetate.

References

1. Saini, V.; Singh, H. Predicting the ET(30) Parameter of Organic Solvents via Machine Learning. *Chemical Physics Letters* **2023**, *826*, 140672, doi:10.1016/j.cplett.2023.140672.