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Machine learning based prediction of luminescence properties of ion-doped Cs_2ZrCl_6 crystalline powders

Lukai Wang*, Shenghong Wang, Longtao Wu, Zhenyu Wang, Zhiyuan Li, Ye Chen and Zungang Wang*

State Key Laboratory of Chemistry for NBC Hazards Protection, Beijing, China

* Correspondence authors; E-mails: wanglukai@sklnbcpc.cn (L.W.); zhigang7991@163.com (Z.W.).

1. Supplementary tables

Table S1. Raw data collected from the literature.

Chemical_Structure	D	D_conc	R	EN	V	M	t	μ	EW	τ	Reference
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.010	0.76	2.05	3	121.76	0.972614311	0.39801105	620	7.20	
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.020	0.76	2.05	3	121.76	0.972460587	0.398232044			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.040	0.76	2.05	3	121.76	0.972153284	0.398674033			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.050	0.76	2.05	3	121.76	0.971999705	0.398895028	625	7.10	
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.060	0.76	2.05	3	121.76	0.971846175	0.399116022			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.080	0.76	2.05	3	121.76	0.971539260	0.399558011			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.090	0.76	2.05	3	121.76	0.971385875	0.399779006			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.100	0.76	2.05	3	121.76	0.971232539	0.400000000	625	7.00	
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.120	0.76	2.05	3	121.76	0.970926011	0.400441989			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.140	0.76	2.05	3	121.76	0.970619677	0.400883978			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.150	0.76	2.05	3	121.76	0.970466582	0.401104972	625	7.10	[1]
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.160	0.76	2.05	3	121.76	0.970313536	0.401325967			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.180	0.76	2.05	3	121.76	0.970007588	0.401767956			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.190	0.76	2.05	3	121.76	0.969854687	0.40198895			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.200	0.76	2.05	3	121.76	0.969701833	0.402209945	625	6.90	
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.220	0.76	2.05	3	121.76	0.969396271	0.402651934			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.240	0.76	2.05	3	121.76	0.969090901	0.403093923			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.260	0.76	2.05	3	121.76	0.968785724	0.403535912			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.280	0.76	2.05	3	121.76	0.968480739	0.403977901			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.300	0.76	2.05	3	121.76	0.968175945	0.404419890	625	6.80	
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.010	0.76	2.05	3	121.76	0.972614311	0.398011050			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.020	0.76	2.05	3	121.76	0.972460587	0.398232044	593	3.06	
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.030	0.76	2.05	3	121.76	0.972306911	0.398453039			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.040	0.76	2.05	3	121.76	0.972153284	0.398674033			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.050	0.76	2.05	3	121.76	0.971999705	0.398895028	592	3.85	[2]
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.060	0.76	2.05	3	121.76	0.971846175	0.399116022			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.070	0.76	2.05	3	121.76	0.971692693	0.399337017			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.080	0.76	2.05	3	121.76	0.971539260	0.399558011			

Table S1. *Cont.*

chemical_structure	D	D_conc	R	EN	V	M	t	μ	EW	τ	Reference
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.090	0.76	2.05	3	121.76	0.971385875	0.399779006			[2]
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.100	0.76	2.05	3	121.76	0.971232539	0.400000000	592	3.95	
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.005	0.76	2.05	3	121.76	0.972691192	0.397900552	592	5.58	
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.010	0.76	2.05	3	121.76	0.972614311	0.398011050	580	5.61	
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.015	0.76	2.05	3	121.76	0.972537443	0.398121547	580	5.62	
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.020	0.76	2.05	3	121.76	0.972460587	0.398232044	580	5.40	
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.025	0.76	2.05	3	121.76	0.972383743	0.398342541			[3]
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.030	0.76	2.05	3	121.76	0.972306911	0.398453039	580	5.34	
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.035	0.76	2.05	3	121.76	0.972230091	0.398563536			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.040	0.76	2.05	3	121.76	0.972153284	0.398674033	580	5.28	
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.045	0.76	2.05	3	121.76	0.972076488	0.398784530			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.050	0.76	2.05	3	121.76	0.971999705	0.398895028	580	5.16	
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.055	0.76	2.05	3	121.76	0.971922934	0.399005525			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.060	0.76	2.05	3	121.76	0.971846175	0.399116022	580	5.02	
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.065	0.76	2.05	3	121.76	0.971769428	0.399226519			
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.080	0.76	2.05	3	121.76	0.971539260	0.399558011	580	4.84	
$Cs_2ZrCl_6:Te^{4+}$	Te	0.0015	0.97	2.1	4	127.6	0.972623921	0.397997238	570	3.70	[4]
$Cs_2ZrCl_6:Te^{4+}$	Te	0.002	0.97	2.1	4	127.6	0.972575876	0.398066298	572.2	2.05	
$Cs_2ZrCl_6:Te^{4+}$	Te	0.003	0.97	2.1	4	127.6	0.972479800	0.398204420	572.2	2.06	
$Cs_2ZrCl_6:Te^{4+}$	Te	0.005	0.97	2.1	4	127.6	0.972287705	0.398480663	572.2	2.50	
$Cs_2ZrCl_6:Te^{4+}$	Te	0.006	0.97	2.1	4	127.6	0.972191686	0.398618785			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.008	0.97	2.1	4	127.6	0.971999705	0.398895028	571.7	1.72	
$Cs_2ZrCl_6:Te^{4+}$	Te	0.010	0.97	2.1	4	127.6	0.971807800	0.399171271			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.012	0.97	2.1	4	127.6	0.971615970	0.399447514			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.013	0.97	2.1	4	127.6	0.971520084	0.399585635			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.014	0.97	2.1	4	127.6	0.971424217	0.399723757			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.016	0.97	2.1	4	127.6	0.971232539	0.400000000			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.018	0.97	2.1	4	127.6	0.971040936	0.400276243			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.020	0.97	2.1	4	127.6	0.970849410	0.400552486			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.021	0.97	2.1	4	127.6	0.970753674	0.400690608	575.5	1.67	
$Cs_2ZrCl_6:Te^{4+}$	Te	0.024	0.97	2.1	4	127.6	0.970466582	0.401104972			[5]
$Cs_2ZrCl_6:Te^{4+}$	Te	0.028	0.97	2.1	4	127.6	0.970084057	0.401657459			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.032	0.97	2.1	4	127.6	0.969701833	0.402209945			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.036	0.97	2.1	4	127.6	0.969319911	0.402762431			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.040	0.97	2.1	4	127.6	0.968938289	0.403314917			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.044	0.97	2.1	4	127.6	0.968556967	0.403867403			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.048	0.97	2.1	4	127.6	0.968175945	0.404419890	573.1	1.33	
$Cs_2ZrCl_6:Te^{4+}$	Te	0.052	0.97	2.1	4	127.6	0.967795223	0.404972376			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.056	0.97	2.1	4	127.6	0.967414801	0.405524862			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.060	0.97	2.1	4	127.6	0.967034677	0.406077348			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.064	0.97	2.1	4	127.6	0.966654852	0.406629834			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.068	0.97	2.1	4	127.6	0.966275325	0.407182320			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.072	0.97	2.1	4	127.6	0.965896096	0.407734807			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.076	0.97	2.1	4	127.6	0.965517165	0.408287293			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.079	0.97	2.1	4	127.6	0.965233161	0.408701657	574.5	1.17	

Table S1. *Cont.*

chemical_structure	D	D_conc	R	EN	V	M	t	μ	EW	τ	Reference
$Cs_2ZrCl_6:Te^{4+}$	Te	0.092	0.97	2.1	4	127.6	0.964004408	0.410497238			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.104	0.97	2.1	4	127.6	0.962872947	0.412154696			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.116	0.97	2.1	4	127.6	0.961744140	0.413812155			[5]
$Cs_2ZrCl_6:Te^{4+}$	Te	0.128	0.97	2.1	4	127.6	0.960617975	0.415469613			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.140	0.97	2.1	4	127.6	0.959494446	0.417127072			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.148	0.97	2.1	4	127.6	0.958746885	0.418232044	575	0.95	
$Cs_2ZrCl_6:Te^{4+}$	Te	0.010	0.97	2.1	4	127.6	0.971807800	0.399171271	572	6.30	
$Cs_2ZrCl_6:Te^{4+}$	Te	0.015	0.97	2.1	4	127.6	0.971328368	0.399861878			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.020	0.97	2.1	4	127.6	0.970849410	0.400552486			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.025	0.97	2.1	4	127.6	0.970370923	0.401243094			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.030	0.97	2.1	4	127.6	0.969892908	0.401933702	572	4.30	
$Cs_2ZrCl_6:Te^{4+}$	Te	0.035	0.97	2.1	4	127.6	0.969415363	0.402624309			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.040	0.97	2.1	4	127.6	0.968938289	0.403314917			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.045	0.97	2.1	4	127.6	0.968461683	0.404005525			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.050	0.97	2.1	4	127.6	0.967985547	0.404696133	574	3.50	[6]
$Cs_2ZrCl_6:Te^{4+}$	Te	0.055	0.97	2.1	4	127.6	0.967509878	0.405386740			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.060	0.97	2.1	4	127.6	0.967034677	0.406077348			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.065	0.97	2.1	4	127.6	0.966559942	0.406767956			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.070	0.97	2.1	4	127.6	0.966085673	0.407458564	575	3.00	
$Cs_2ZrCl_6:Te^{4+}$	Te	0.075	0.97	2.1	4	127.6	0.965611870	0.408149171			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.080	0.97	2.1	4	127.6	0.965138531	0.408839779			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.085	0.97	2.1	4	127.6	0.964665655	0.409530387			
$Cs_2ZrCl_6:Te^{4+}$	Te	0.090	0.97	2.1	4	127.6	0.964193243	0.410220994	576	2.70	
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.025	0.615	1.66	3	51.996	0.973778427	0.396339779	903.5	35.01	
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.028	0.615	1.66	3	51.996	0.973899810	0.396165746			
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.03	0.615	1.66	3	51.996	0.973980748	0.396049724			
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.034	0.615	1.66	3	51.996	0.974142665	0.395817680			
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.038	0.615	1.66	3	51.996	0.974304636	0.395585635			
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.042	0.615	1.66	3	51.996	0.974466661	0.395353591			
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.046	0.615	1.66	3	51.996	0.974628739	0.395121547			
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.050	0.615	1.66	3	51.996	0.974790872	0.394889503	900.3	34.70	
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.054	0.615	1.66	3	51.996	0.974953058	0.394657459			
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.058	0.615	1.66	3	51.996	0.975115299	0.394425414			
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.062	0.615	1.66	3	51.996	0.975277593	0.394193370			
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.066	0.615	1.66	3	51.996	0.975439941	0.393961326			[7]
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.070	0.615	1.66	3	51.996	0.975602344	0.393729282			
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.078	0.615	1.66	3	51.996	0.975927311	0.393265193			
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.086	0.615	1.66	3	51.996	0.976252495	0.392801105			
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.094	0.615	1.66	3	51.996	0.976577896	0.392337017			
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.100	0.615	1.66	3	51.996	0.976822089	0.391988950	897.1	32.93	
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.120	0.615	1.66	3	51.996	0.977636948	0.390828729			
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.140	0.615	1.66	3	51.996	0.978453168	0.389668508			
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.160	0.615	1.66	3	51.996	0.979270752	0.388508287			
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.180	0.615	1.66	3	51.996	0.980089703	0.387348066			
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.200	0.615	1.66	3	51.996	0.980910025	0.386187845	900.3	30.83	
$Cs_2ZrCl_6: Cr^{3+}$	Cr	0.220	0.615	1.66	3	51.996	0.981731722	0.385027624			

Table S1. *Cont.*

chemical_structure	D	D_conc	R	EN	V	M	t	μ	EW	τ	Reference
Cs_2ZrCl_6: Cr^{3+}	Cr	0.240	0.615	1.66	3	51.996	0.982554796	0.383867403			
Cs_2ZrCl_6: Cr^{3+}	Cr	0.260	0.615	1.66	3	51.996	0.983379252	0.382707182			
Cs_2ZrCl_6: Cr^{3+}	Cr	0.280	0.615	1.66	3	51.996	0.984205092	0.381546961			
Cs_2ZrCl_6: Cr^{3+}	Cr	0.300	0.615	1.66	3	51.996	0.985032321	0.380386740			
Cs_2ZrCl_6: Cr^{3+}	Cr	0.320	0.615	1.66	3	51.996	0.985860941	0.379226519			[7]
Cs_2ZrCl_6: Cr^{3+}	Cr	0.340	0.615	1.66	3	51.996	0.986690957	0.378066298			
Cs_2ZrCl_6: Cr^{3+}	Cr	0.360	0.615	1.66	3	51.996	0.987522371	0.376906077			
Cs_2ZrCl_6: Cr^{3+}	Cr	0.380	0.615	1.66	3	51.996	0.988355188	0.375745856			
Cs_2ZrCl_6: Cr^{3+}	Cr	0.400	0.615	1.66	3	51.996	0.989189410	0.374585635	893.9	24.81	
Cs_2ZrCl_6: Mn^{2+}	Mn	0.050	0.83	1.55	2	54.94	0.970657958	0.400828729	444.2	12.60	
Cs_2ZrCl_6: Mn^{2+}	Mn	0.060	0.83	1.55	2	54.94	0.970237031	0.401436464			
Cs_2ZrCl_6: Mn^{2+}	Mn	0.070	0.83	1.55	2	54.94	0.969816469	0.402044199			
Cs_2ZrCl_6: Mn^{2+}	Mn	0.080	0.83	1.55	2	54.94	0.969396271	0.402651934			
Cs_2ZrCl_6: Mn^{2+}	Mn	0.090	0.83	1.55	2	54.94	0.968976437	0.403259669			
Cs_2ZrCl_6: Mn^{2+}	Mn	0.100	0.83	1.55	2	54.94	0.968556967	0.403867403	444.6	12.80	
Cs_2ZrCl_6: Mn^{2+}	Mn	0.120	0.83	1.55	2	54.94	0.967719115	0.405082873			
Cs_2ZrCl_6: Mn^{2+}	Mn	0.140	0.83	1.55	2	54.94	0.966882711	0.406298343			
Cs_2ZrCl_6: Mn^{2+}	Mn	0.160	0.83	1.55	2	54.94	0.966047752	0.407513812			
Cs_2ZrCl_6: Mn^{2+}	Mn	0.180	0.83	1.55	2	54.94	0.965214234	0.408729282			
Cs_2ZrCl_6: Mn^{2+}	Mn	0.200	0.83	1.55	2	54.94	0.964382153	0.409944751	444.8	13.00	[8]
Cs_2ZrCl_6: Mn^{2+}	Mn	0.220	0.83	1.55	2	54.94	0.963551505	0.411160221			
Cs_2ZrCl_6: Mn^{2+}	Mn	0.240	0.83	1.55	2	54.94	0.962722286	0.412375691			
Cs_2ZrCl_6: Mn^{2+}	Mn	0.260	0.83	1.55	2	54.94	0.961894494	0.413591160			
Cs_2ZrCl_6: Mn^{2+}	Mn	0.280	0.83	1.55	2	54.94	0.961068124	0.414806630			
Cs_2ZrCl_6: Mn^{2+}	Mn	0.300	0.83	1.55	2	54.94	0.960243173	0.416022099			
Cs_2ZrCl_6: Mn^{2+}	Mn	0.320	0.83	1.55	2	54.94	0.959419637	0.417237569			
Cs_2ZrCl_6: Mn^{2+}	Mn	0.340	0.83	1.55	2	54.94	0.958597512	0.418453039			
Cs_2ZrCl_6: Mn^{2+}	Mn	0.360	0.83	1.55	2	54.94	0.957776795	0.419668508			
Cs_2ZrCl_6: Mn^{2+}	Mn	0.380	0.83	1.55	2	54.94	0.956957482	0.420883978			
Cs_2ZrCl_6: Mn^{2+}	Mn	0.400	0.83	1.55	2	54.94	0.956139570	0.422099448	444.9	12.90	
Cs_2ZrCl_6: Mo^{4+}	Mo	0.030	0.65	2.16	4	95.95	0.973576191	0.396629834	911	11.60	
Cs_2ZrCl_6: Mo^{4+}	Mo	0.040	0.65	2.16	4	95.95	0.973845858	0.396243094			
Cs_2ZrCl_6: Mo^{4+}	Mo	0.060	0.65	2.16	4	95.95	0.974385641	0.395469613			
Cs_2ZrCl_6: Mo^{4+}	Mo	0.080	0.65	2.16	4	95.95	0.974926023	0.394696133			
Cs_2ZrCl_6: Mo^{4+}	Mo	0.100	0.65	2.16	4	95.95	0.975467005	0.393922652			
Cs_2ZrCl_6: Mo^{4+}	Mo	0.120	0.65	2.16	4	95.95	0.976008587	0.393149171			
Cs_2ZrCl_6: Mo^{4+}	Mo	0.140	0.65	2.16	4	95.95	0.976550771	0.392375691			
Cs_2ZrCl_6: Mo^{4+}	Mo	0.150	0.65	2.16	4	95.95	0.976822089	0.391988950	917	9.80	[9]
Cs_2ZrCl_6: Mo^{4+}	Mo	0.160	0.65	2.16	4	95.95	0.977093558	0.391602210			
Cs_2ZrCl_6: Mo^{4+}	Mo	0.200	0.65	2.16	4	95.95	0.978180943	0.390055249			
Cs_2ZrCl_6: Mo^{4+}	Mo	0.240	0.65	2.16	4	95.95	0.979270752	0.388508287			
Cs_2ZrCl_6: Mo^{4+}	Mo	0.280	0.65	2.16	4	95.95	0.980362991	0.386961326			
Cs_2ZrCl_6: Mo^{4+}	Mo	0.320	0.65	2.16	4	95.95	0.981457670	0.385414365			
Cs_2ZrCl_6: Mo^{4+}	Mo	0.360	0.65	2.16	4	95.95	0.982554796	0.383867403			
Cs_2ZrCl_6: Mo^{4+}	Mo	0.400	0.65	2.16	4	95.95	0.983654378	0.382320442			
Cs_2ZrCl_6: Mo^{4+}	Mo	0.440	0.65	2.16	4	95.95	0.984756423	0.380773481			

Table S1. *Cont.*

chemical_structure	D	D_conc	R	EN	V	M	t	μ	EW	τ	Reference
Cs_2ZrCl_6: Mo^{4+}	Mo	0.480	0.65	2.16	4	95.95	0.985860941	0.379226519			[9]
Cs_2ZrCl_6: Mo^{4+}	Mo	0.500	0.65	2.16	4	95.95	0.986414130	0.378453039	921	4.30	
Cs_2ZrCl_6:Bi^{3+}	Bi	0.000	1.03	2.02	3	208.98	0.972768084	0.397790055	465	1.78	
Cs_2ZrCl_6:Bi^{3+}	Bi	0.005	1.03	2.02	3	208.98	0.972172485	0.398646409			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.010	1.03	2.02	3	208.98	0.971577614	0.399502762			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.014	1.03	2.02	3	208.98	0.971102241	0.400187845			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.018	1.03	2.02	3	208.98	0.970627333	0.400872928			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.020	1.03	2.02	3	208.98	0.970390053	0.401215470	465		
Cs_2ZrCl_6:Bi^{3+}	Bi	0.024	1.03	2.02	3	208.98	0.969915842	0.401900552			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.028	1.03	2.02	3	208.98	0.969442093	0.402585635			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.032	1.03	2.02	3	208.98	0.968968807	0.403270718			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.036	1.03	2.02	3	208.98	0.968495983	0.403955801			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.040	1.03	2.02	3	208.98	0.968023621	0.404640884	465		
Cs_2ZrCl_6:Bi^{3+}	Bi	0.044	1.03	2.02	3	208.98	0.967551718	0.405325967			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.048	1.03	2.02	3	208.98	0.967080276	0.406011050			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.052	1.03	2.02	3	208.98	0.966609293	0.406696133			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.056	1.03	2.02	3	208.98	0.966138768	0.407381215			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.060	1.03	2.02	3	208.98	0.965668702	0.408066298	465	2.08	
Cs_2ZrCl_6:Bi^{3+}	Bi	0.062	1.03	2.02	3	208.98	0.965433840	0.408408840			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.064	1.03	2.02	3	208.98	0.965199092	0.408751381			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.066	1.03	2.02	3	208.98	0.964964459	0.409093923			[10]
Cs_2ZrCl_6:Bi^{3+}	Bi	0.068	1.03	2.02	3	208.98	0.964729939	0.409436464			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.070	1.03	2.02	3	208.98	0.964495534	0.409779006			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.072	1.03	2.02	3	208.98	0.964261242	0.410121547			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.074	1.03	2.02	3	208.98	0.964027064	0.410464088			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.076	1.03	2.02	3	208.98	0.963793000	0.410806630			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.078	1.03	2.02	3	208.98	0.963559050	0.411149171			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.080	1.03	2.02	3	208.98	0.963325213	0.411491713	465		
Cs_2ZrCl_6:Bi^{3+}	Bi	0.082	1.03	2.02	3	208.98	0.963091489	0.411834254			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.086	1.03	2.02	3	208.98	0.962624382	0.412519337			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.090	1.03	2.02	3	208.98	0.962157728	0.413204420			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.094	1.03	2.02	3	208.98	0.961691527	0.413889503			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.098	1.03	2.02	3	208.98	0.961225776	0.414574586			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.100	1.03	2.02	3	208.98	0.960993070	0.414917127	465		
Cs_2ZrCl_6:Bi^{3+}	Bi	0.104	1.03	2.02	3	208.98	0.960527996	0.415602210			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.108	1.03	2.02	3	208.98	0.960063372	0.416287293			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.112	1.03	2.02	3	208.98	0.959599197	0.416972376			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.116	1.03	2.02	3	208.98	0.959135471	0.417657459			
Cs_2ZrCl_6:Bi^{3+}	Bi	0.120	1.03	2.02	3	208.98	0.958672193	0.418342541	465	2.56	

Empty values indicate the unavailability of corresponding data.

Table S2. Data supplemented by interpolation.

chemical_structure	D	D_conc	R	EN	V	M	t	μ	EW	τ
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.010	0.76	2.05	3	121.76	0.9726	0.3980	620	7.20
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.020	0.76	2.05	3	121.76	0.9725	0.3982	622	7.17
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.040	0.76	2.05	3	121.76	0.9722	0.3987	623	7.13
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.050	0.76	2.05	3	121.76	0.9720	0.3989	625	7.10
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.060	0.76	2.05	3	121.76	0.9718	0.3991	625	7.08
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.080	0.76	2.05	3	121.76	0.9715	0.3996	625	7.05
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.090	0.76	2.05	3	121.76	0.9714	0.3998	625	7.03
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.100	0.76	2.05	3	121.76	0.9712	0.4000	625	7.00
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.120	0.76	2.05	3	121.76	0.9709	0.4004	625	7.03
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.140	0.76	2.05	3	121.76	0.9706	0.4009	625	7.07
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.150	0.76	2.05	3	121.76	0.9705	0.4011	625	7.10
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.160	0.76	2.05	3	121.76	0.9703	0.4013	625	7.05
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.180	0.76	2.05	3	121.76	0.9700	0.4018	625	7.00
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.190	0.76	2.05	3	121.76	0.9699	0.4020	625	6.95
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.200	0.76	2.05	3	121.76	0.9697	0.4022	625	6.90
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.220	0.76	2.05	3	121.76	0.9694	0.4027	625	6.88
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.240	0.76	2.05	3	121.76	0.9691	0.4031	625	6.86
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.260	0.76	2.05	3	121.76	0.9688	0.4035	625	6.84
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.280	0.76	2.05	3	121.76	0.9685	0.4040	625	6.82
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.300	0.76	2.05	3	121.76	0.9682	0.4044	625	6.80
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.010	0.76	2.05	3	121.76	0.9726	0.3980	609	4.93
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.020	0.76	2.05	3	121.76	0.9725	0.3982	593	3.06
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.030	0.76	2.05	3	121.76	0.9723	0.3985	593	3.32
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.040	0.76	2.05	3	121.76	0.9722	0.3987	592	3.59
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.050	0.76	2.05	3	121.76	0.9720	0.3989	592	3.85
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.060	0.76	2.05	3	121.76	0.9718	0.3991	592	3.87
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.070	0.76	2.05	3	121.76	0.9717	0.3993	592	3.89
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.080	0.76	2.05	3	121.76	0.9715	0.3996	592	3.91
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.090	0.76	2.05	3	121.76	0.9714	0.3998	592	3.93
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.100	0.76	2.05	3	121.76	0.9712	0.4000	592	3.95
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.005	0.76	2.05	3	121.76	0.9727	0.3979	592	5.58
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.010	0.76	2.05	3	121.76	0.9726	0.3980	580	5.61
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.015	0.76	2.05	3	121.76	0.9725	0.3981	580	5.62
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.020	0.76	2.05	3	121.76	0.9725	0.3982	580	5.40
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.025	0.76	2.05	3	121.76	0.9724	0.3983	580	5.37
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.030	0.76	2.05	3	121.76	0.9723	0.3985	580	5.34
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.035	0.76	2.05	3	121.76	0.9722	0.3986	580	5.31
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.040	0.76	2.05	3	121.76	0.9722	0.3987	580	5.28
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.045	0.76	2.05	3	121.76	0.9721	0.3988	580	5.22
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.050	0.76	2.05	3	121.76	0.9720	0.3989	580	5.16
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.055	0.76	2.05	3	121.76	0.9719	0.3990	580	5.09
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.060	0.76	2.05	3	121.76	0.9718	0.3991	580	5.02
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.065	0.76	2.05	3	121.76	0.9718	0.3992	580	4.93
$Cs_2ZrCl_6:Sb^{3+}$	Sb	0.080	0.76	2.05	3	121.76	0.9715	0.3996	580	4.84
$Cs_2ZrCl_6:Te^{4+}$	Te	0.002	0.97	2.1	4	127.6	0.9726	0.3980	570	3.70
$Cs_2ZrCl_6:Te^{4+}$	Te	0.002	0.97	2.1	4	127.6	0.9726	0.3981	572	2.05
$Cs_2ZrCl_6:Te^{4+}$	Te	0.003	0.97	2.1	4	127.6	0.9725	0.3982	572	2.06
$Cs_2ZrCl_6:Te^{4+}$	Te	0.005	0.97	2.1	4	127.6	0.9723	0.3985	572	2.50

Table S2. *Cont.*

chemical_structure	D	D_conc	R	EN	V	M	t	μ	EW	τ
$Cs_2ZrCl_6:Te^{4+}$	Te	0.006	0.97	2.1	4	127.6	0.9722	0.3986	572	2.11
$Cs_2ZrCl_6:Te^{4+}$	Te	0.008	0.97	2.1	4	127.6	0.9720	0.3989	572	1.72
$Cs_2ZrCl_6:Te^{4+}$	Te	0.010	0.97	2.1	4	127.6	0.9718	0.3992	572	1.71
$Cs_2ZrCl_6:Te^{4+}$	Te	0.012	0.97	2.1	4	127.6	0.9716	0.3994	573	1.71
$Cs_2ZrCl_6:Te^{4+}$	Te	0.013	0.97	2.1	4	127.6	0.9715	0.3996	573	1.70
$Cs_2ZrCl_6:Te^{4+}$	Te	0.014	0.97	2.1	4	127.6	0.9714	0.3997	574	1.70
$Cs_2ZrCl_6:Te^{4+}$	Te	0.016	0.97	2.1	4	127.6	0.9712	0.4000	574	1.69
$Cs_2ZrCl_6:Te^{4+}$	Te	0.018	0.97	2.1	4	127.6	0.9710	0.4003	575	1.68
$Cs_2ZrCl_6:Te^{4+}$	Te	0.020	0.97	2.1	4	127.6	0.9708	0.4006	575	1.68
$Cs_2ZrCl_6:Te^{4+}$	Te	0.021	0.97	2.1	4	127.6	0.9708	0.4007	576	1.67
$Cs_2ZrCl_6:Te^{4+}$	Te	0.024	0.97	2.1	4	127.6	0.9705	0.4011	575	1.62
$Cs_2ZrCl_6:Te^{4+}$	Te	0.028	0.97	2.1	4	127.6	0.9701	0.4017	575	1.57
$Cs_2ZrCl_6:Te^{4+}$	Te	0.032	0.97	2.1	4	127.6	0.9697	0.4022	574	1.52
$Cs_2ZrCl_6:Te^{4+}$	Te	0.036	0.97	2.1	4	127.6	0.9693	0.4028	574	1.48
$Cs_2ZrCl_6:Te^{4+}$	Te	0.040	0.97	2.1	4	127.6	0.9689	0.4033	574	1.43
$Cs_2ZrCl_6:Te^{4+}$	Te	0.044	0.97	2.1	4	127.6	0.9686	0.4039	573	1.38
$Cs_2ZrCl_6:Te^{4+}$	Te	0.048	0.97	2.1	4	127.6	0.9682	0.4044	573	1.33
$Cs_2ZrCl_6:Te^{4+}$	Te	0.052	0.97	2.1	4	127.6	0.9678	0.4050	573	1.31
$Cs_2ZrCl_6:Te^{4+}$	Te	0.056	0.97	2.1	4	127.6	0.9674	0.4055	573	1.29
$Cs_2ZrCl_6:Te^{4+}$	Te	0.060	0.97	2.1	4	127.6	0.9670	0.4061	574	1.27
$Cs_2ZrCl_6:Te^{4+}$	Te	0.064	0.97	2.1	4	127.6	0.9667	0.4066	574	1.25
$Cs_2ZrCl_6:Te^{4+}$	Te	0.068	0.97	2.1	4	127.6	0.9663	0.4072	574	1.23
$Cs_2ZrCl_6:Te^{4+}$	Te	0.072	0.97	2.1	4	127.6	0.9659	0.4077	574	1.21
$Cs_2ZrCl_6:Te^{4+}$	Te	0.076	0.97	2.1	4	127.6	0.9655	0.4083	574	1.19
$Cs_2ZrCl_6:Te^{4+}$	Te	0.079	0.97	2.1	4	127.6	0.9652	0.4087	575	1.17
$Cs_2ZrCl_6:Te^{4+}$	Te	0.092	0.97	2.1	4	127.6	0.9640	0.4105	575	1.13
$Cs_2ZrCl_6:Te^{4+}$	Te	0.104	0.97	2.1	4	127.6	0.9629	0.4122	575	1.10
$Cs_2ZrCl_6:Te^{4+}$	Te	0.116	0.97	2.1	4	127.6	0.9617	0.4138	575	1.06
$Cs_2ZrCl_6:Te^{4+}$	Te	0.128	0.97	2.1	4	127.6	0.9606	0.4155	575	1.02
$Cs_2ZrCl_6:Te^{4+}$	Te	0.140	0.97	2.1	4	127.6	0.9595	0.4171	575	0.99
$Cs_2ZrCl_6:Te^{4+}$	Te	0.148	0.97	2.1	4	127.6	0.9587	0.4182	575	0.95
$Cs_2ZrCl_6:Te^{4+}$	Te	0.010	0.97	2.1	4	127.6	0.9718	0.3992	572	6.30
$Cs_2ZrCl_6:Te^{4+}$	Te	0.015	0.97	2.1	4	127.6	0.9713	0.3999	572	5.80
$Cs_2ZrCl_6:Te^{4+}$	Te	0.020	0.97	2.1	4	127.6	0.9708	0.4006	572	5.30
$Cs_2ZrCl_6:Te^{4+}$	Te	0.025	0.97	2.1	4	127.6	0.9704	0.4012	572	4.80
$Cs_2ZrCl_6:Te^{4+}$	Te	0.030	0.97	2.1	4	127.6	0.9699	0.4019	572	4.30
$Cs_2ZrCl_6:Te^{4+}$	Te	0.035	0.97	2.1	4	127.6	0.9694	0.4026	573	4.10
$Cs_2ZrCl_6:Te^{4+}$	Te	0.040	0.97	2.1	4	127.6	0.9689	0.4033	573	3.90
$Cs_2ZrCl_6:Te^{4+}$	Te	0.045	0.97	2.1	4	127.6	0.9685	0.4040	574	3.70
$Cs_2ZrCl_6:Te^{4+}$	Te	0.050	0.97	2.1	4	127.6	0.9680	0.4047	574	3.50
$Cs_2ZrCl_6:Te^{4+}$	Te	0.055	0.97	2.1	4	127.6	0.9675	0.4054	574	3.38
$Cs_2ZrCl_6:Te^{4+}$	Te	0.060	0.97	2.1	4	127.6	0.9670	0.4061	575	3.25
$Cs_2ZrCl_6:Te^{4+}$	Te	0.065	0.97	2.1	4	127.6	0.9666	0.4068	575	3.13
$Cs_2ZrCl_6:Te^{4+}$	Te	0.070	0.97	2.1	4	127.6	0.9661	0.4075	575	3.00
$Cs_2ZrCl_6:Te^{4+}$	Te	0.075	0.97	2.1	4	127.6	0.9656	0.4081	575	2.93
$Cs_2ZrCl_6:Te^{4+}$	Te	0.080	0.97	2.1	4	127.6	0.9651	0.4088	576	2.85
$Cs_2ZrCl_6:Te^{4+}$	Te	0.085	0.97	2.1	4	127.6	0.9647	0.4095	576	2.78
$Cs_2ZrCl_6:Te^{4+}$	Te	0.090	0.97	2.1	4	127.6	0.9642	0.4102	576	2.70

Table S2. *Cont.*

chemical_structure	D	D_conc	R	EN	V	M	t	μ	EW	τ
Cs_2ZrCl_6: Cr^{3+}	Cr	0.025	0.615	1.66	3	51.996	0.9738	0.3963	904	35.01
Cs_2ZrCl_6: Cr^{3+}	Cr	0.028	0.615	1.66	3	51.996	0.9739	0.3962	903	34.97
Cs_2ZrCl_6: Cr^{3+}	Cr	0.030	0.615	1.66	3	51.996	0.9740	0.3960	903	34.92
Cs_2ZrCl_6: Cr^{3+}	Cr	0.034	0.615	1.66	3	51.996	0.9741	0.3958	902	34.88
Cs_2ZrCl_6: Cr^{3+}	Cr	0.038	0.615	1.66	3	51.996	0.9743	0.3956	902	34.83
Cs_2ZrCl_6: Cr^{3+}	Cr	0.042	0.615	1.66	3	51.996	0.9745	0.3954	901	34.79
Cs_2ZrCl_6: Cr^{3+}	Cr	0.046	0.615	1.66	3	51.996	0.9746	0.3951	901	34.74
Cs_2ZrCl_6: Cr^{3+}	Cr	0.050	0.615	1.66	3	51.996	0.9748	0.3949	900	34.70
Cs_2ZrCl_6: Cr^{3+}	Cr	0.054	0.615	1.66	3	51.996	0.9750	0.3947	900	34.50
Cs_2ZrCl_6: Cr^{3+}	Cr	0.058	0.615	1.66	3	51.996	0.9751	0.3944	900	34.31
Cs_2ZrCl_6: Cr^{3+}	Cr	0.062	0.615	1.66	3	51.996	0.9753	0.3942	899	34.11
Cs_2ZrCl_6: Cr^{3+}	Cr	0.066	0.615	1.66	3	51.996	0.9754	0.3940	899	33.91
Cs_2ZrCl_6: Cr^{3+}	Cr	0.070	0.615	1.66	3	51.996	0.9756	0.3937	899	33.72
Cs_2ZrCl_6: Cr^{3+}	Cr	0.078	0.615	1.66	3	51.996	0.9759	0.3933	898	33.52
Cs_2ZrCl_6: Cr^{3+}	Cr	0.086	0.615	1.66	3	51.996	0.9763	0.3928	898	33.32
Cs_2ZrCl_6: Cr^{3+}	Cr	0.094	0.615	1.66	3	51.996	0.9766	0.3923	897	33.13
Cs_2ZrCl_6: Cr^{3+}	Cr	0.100	0.615	1.66	3	51.996	0.9768	0.3920	897	32.93
Cs_2ZrCl_6: Cr^{3+}	Cr	0.120	0.615	1.66	3	51.996	0.9776	0.3908	898	32.51
Cs_2ZrCl_6: Cr^{3+}	Cr	0.140	0.615	1.66	3	51.996	0.9785	0.3897	898	32.09
Cs_2ZrCl_6: Cr^{3+}	Cr	0.160	0.615	1.66	3	51.996	0.9793	0.3885	899	31.67
Cs_2ZrCl_6: Cr^{3+}	Cr	0.180	0.615	1.66	3	51.996	0.9801	0.3873	900	31.25
Cs_2ZrCl_6: Cr^{3+}	Cr	0.200	0.615	1.66	3	51.996	0.9809	0.3862	900	30.83
Cs_2ZrCl_6: Cr^{3+}	Cr	0.220	0.615	1.66	3	51.996	0.9817	0.3850	900	30.23
Cs_2ZrCl_6: Cr^{3+}	Cr	0.240	0.615	1.66	3	51.996	0.9826	0.3839	899	29.63
Cs_2ZrCl_6: Cr^{3+}	Cr	0.260	0.615	1.66	3	51.996	0.9834	0.3827	898	29.02
Cs_2ZrCl_6: Cr^{3+}	Cr	0.280	0.615	1.66	3	51.996	0.9842	0.3815	898	28.42
Cs_2ZrCl_6: Cr^{3+}	Cr	0.300	0.615	1.66	3	51.996	0.9850	0.3804	897	27.82
Cs_2ZrCl_6: Cr^{3+}	Cr	0.320	0.615	1.66	3	51.996	0.9859	0.3792	896	27.22
Cs_2ZrCl_6: Cr^{3+}	Cr	0.340	0.615	1.66	3	51.996	0.9867	0.3781	896	26.62
Cs_2ZrCl_6: Cr^{3+}	Cr	0.360	0.615	1.66	3	51.996	0.9875	0.3769	895	26.01
Cs_2ZrCl_6: Cr^{3+}	Cr	0.380	0.615	1.66	3	51.996	0.9884	0.3757	895	25.41
Cs_2ZrCl_6: Cr^{3+}	Cr	0.400	0.615	1.66	3	51.996	0.9892	0.3746	894	24.81
Cs_2ZrCl_6: Mn^{2+}	Mn	0.050	0.83	1.55	2	54.94	0.9707	0.4008	444	12.60
Cs_2ZrCl_6: Mn^{2+}	Mn	0.060	0.83	1.55	2	54.94	0.9702	0.4014	444	12.64
Cs_2ZrCl_6: Mn^{2+}	Mn	0.070	0.83	1.55	2	54.94	0.9698	0.4020	444	12.68
Cs_2ZrCl_6: Mn^{2+}	Mn	0.080	0.83	1.55	2	54.94	0.9694	0.4027	444	12.72
Cs_2ZrCl_6: Mn^{2+}	Mn	0.090	0.83	1.55	2	54.94	0.9690	0.4033	445	12.76
Cs_2ZrCl_6: Mn^{2+}	Mn	0.100	0.83	1.55	2	54.94	0.9686	0.4039	445	12.80
Cs_2ZrCl_6: Mn^{2+}	Mn	0.120	0.83	1.55	2	54.94	0.9677	0.4051	445	12.84
Cs_2ZrCl_6: Mn^{2+}	Mn	0.140	0.83	1.55	2	54.94	0.9669	0.4063	445	12.88
Cs_2ZrCl_6: Mn^{2+}	Mn	0.160	0.83	1.55	2	54.94	0.9660	0.4075	445	12.92
Cs_2ZrCl_6: Mn^{2+}	Mn	0.180	0.83	1.55	2	54.94	0.9652	0.4087	445	12.96
Cs_2ZrCl_6: Mn^{2+}	Mn	0.200	0.83	1.55	2	54.94	0.9644	0.4099	445	13.00
Cs_2ZrCl_6: Mn^{2+}	Mn	0.220	0.83	1.55	2	54.94	0.9636	0.4112	445	12.99
Cs_2ZrCl_6: Mn^{2+}	Mn	0.240	0.83	1.55	2	54.94	0.9627	0.4124	445	12.98
Cs_2ZrCl_6: Mn^{2+}	Mn	0.260	0.83	1.55	2	54.94	0.9619	0.4136	445	12.97
Cs_2ZrCl_6: Mn^{2+}	Mn	0.280	0.83	1.55	2	54.94	0.9611	0.4148	445	12.96
Cs_2ZrCl_6: Mn^{2+}	Mn	0.300	0.83	1.55	2	54.94	0.9602	0.4160	445	12.95

Table S2. *Cont.*

chemical_structure	D	D_conc	R	EN	V	M	t	μ	EW	τ
Cs_2ZrCl_6: Mn^{2+}	Mn	0.320	0.83	1.55	2	54.94	0.9594	0.4172	445	12.94
Cs_2ZrCl_6: Mn^{2+}	Mn	0.340	0.83	1.55	2	54.94	0.9586	0.4185	445	12.93
Cs_2ZrCl_6: Mn^{2+}	Mn	0.360	0.83	1.55	2	54.94	0.9578	0.4197	445	12.92
Cs_2ZrCl_6: Mn^{2+}	Mn	0.380	0.83	1.55	2	54.94	0.9570	0.4209	445	12.91
Cs_2ZrCl_6: Mn^{2+}	Mn	0.400	0.83	1.55	2	54.94	0.9561	0.4221	445	12.90
Cs_2ZrCl_6: Mo^{4+}	Mo	0.030	0.65	2.16	4	95.95	0.9736	0.3966	911	11.60
Cs_2ZrCl_6: Mo^{4+}	Mo	0.040	0.65	2.16	4	95.95	0.9738	0.3962	912	11.34
Cs_2ZrCl_6: Mo^{4+}	Mo	0.060	0.65	2.16	4	95.95	0.9744	0.3955	913	11.09
Cs_2ZrCl_6: Mo^{4+}	Mo	0.080	0.65	2.16	4	95.95	0.9749	0.3947	914	10.83
Cs_2ZrCl_6: Mo^{4+}	Mo	0.100	0.65	2.16	4	95.95	0.9755	0.3939	914	10.57
Cs_2ZrCl_6: Mo^{4+}	Mo	0.120	0.65	2.16	4	95.95	0.9760	0.3931	915	10.31
Cs_2ZrCl_6: Mo^{4+}	Mo	0.140	0.65	2.16	4	95.95	0.9766	0.3924	916	10.06
Cs_2ZrCl_6: Mo^{4+}	Mo	0.150	0.65	2.16	4	95.95	0.9768	0.3920	917	9.80
Cs_2ZrCl_6: Mo^{4+}	Mo	0.160	0.65	2.16	4	95.95	0.9771	0.3916	917	9.25
Cs_2ZrCl_6: Mo^{4+}	Mo	0.200	0.65	2.16	4	95.95	0.9782	0.3901	918	8.70
Cs_2ZrCl_6: Mo^{4+}	Mo	0.240	0.65	2.16	4	95.95	0.9793	0.3885	918	8.15
Cs_2ZrCl_6: Mo^{4+}	Mo	0.280	0.65	2.16	4	95.95	0.9804	0.3870	919	7.60
Cs_2ZrCl_6: Mo^{4+}	Mo	0.320	0.65	2.16	4	95.95	0.9815	0.3854	919	7.05
Cs_2ZrCl_6: Mo^{4+}	Mo	0.360	0.65	2.16	4	95.95	0.9826	0.3839	919	6.50
Cs_2ZrCl_6: Mo^{4+}	Mo	0.400	0.65	2.16	4	95.95	0.9837	0.3823	920	5.95
Cs_2ZrCl_6: Mo^{4+}	Mo	0.440	0.65	2.16	4	95.95	0.9848	0.3808	920	5.40
Cs_2ZrCl_6: Mo^{4+}	Mo	0.480	0.65	2.16	4	95.95	0.9859	0.3792	921	4.85
Cs_2ZrCl_6: Mo^{4+}	Mo	0.500	0.65	2.16	4	95.95	0.9864	0.3785	921	4.30
Cs_2ZrCl_6:Bi^{3+}	Bi	0.000	1.03	2.02	3	208.98	0.9728	0.3978	465	1.78
Cs_2ZrCl_6:Bi^{3+}	Bi	0.005	1.03	2.02	3	208.98	0.9722	0.3986	465	1.80
Cs_2ZrCl_6:Bi^{3+}	Bi	0.010	1.03	2.02	3	208.98	0.9716	0.3995	465	1.82
Cs_2ZrCl_6:Bi^{3+}	Bi	0.014	1.03	2.02	3	208.98	0.9711	0.4002	465	1.84
Cs_2ZrCl_6:Bi^{3+}	Bi	0.018	1.03	2.02	3	208.98	0.9706	0.4009	465	1.86
Cs_2ZrCl_6:Bi^{3+}	Bi	0.020	1.03	2.02	3	208.98	0.9704	0.4012	465	1.88
Cs_2ZrCl_6:Bi^{3+}	Bi	0.024	1.03	2.02	3	208.98	0.9699	0.4019	465	1.90
Cs_2ZrCl_6:Bi^{3+}	Bi	0.028	1.03	2.02	3	208.98	0.9694	0.4026	465	1.92
Cs_2ZrCl_6:Bi^{3+}	Bi	0.032	1.03	2.02	3	208.98	0.9690	0.4033	465	1.94
Cs_2ZrCl_6:Bi^{3+}	Bi	0.036	1.03	2.02	3	208.98	0.9685	0.4040	465	1.96
Cs_2ZrCl_6:Bi^{3+}	Bi	0.040	1.03	2.02	3	208.98	0.9680	0.4046	465	1.98
Cs_2ZrCl_6:Bi^{3+}	Bi	0.044	1.03	2.02	3	208.98	0.9676	0.4053	465	2.00
Cs_2ZrCl_6:Bi^{3+}	Bi	0.048	1.03	2.02	3	208.98	0.9671	0.4060	465	2.02
Cs_2ZrCl_6:Bi^{3+}	Bi	0.052	1.03	2.02	3	208.98	0.9666	0.4067	465	2.04
Cs_2ZrCl_6:Bi^{3+}	Bi	0.056	1.03	2.02	3	208.98	0.9661	0.4074	465	2.06
Cs_2ZrCl_6:Bi^{3+}	Bi	0.060	1.03	2.02	3	208.98	0.9657	0.4081	465	2.08
Cs_2ZrCl_6:Bi^{3+}	Bi	0.062	1.03	2.02	3	208.98	0.9654	0.4084	465	2.10
Cs_2ZrCl_6:Bi^{3+}	Bi	0.064	1.03	2.02	3	208.98	0.9652	0.4088	465	2.13
Cs_2ZrCl_6:Bi^{3+}	Bi	0.066	1.03	2.02	3	208.98	0.9650	0.4091	465	2.15
Cs_2ZrCl_6:Bi^{3+}	Bi	0.068	1.03	2.02	3	208.98	0.9647	0.4094	465	2.17
Cs_2ZrCl_6:Bi^{3+}	Bi	0.070	1.03	2.02	3	208.98	0.9645	0.4098	465	2.19
Cs_2ZrCl_6:Bi^{3+}	Bi	0.072	1.03	2.02	3	208.98	0.9643	0.4101	465	2.22
Cs_2ZrCl_6:Bi^{3+}	Bi	0.074	1.03	2.02	3	208.98	0.9640	0.4105	465	2.24
Cs_2ZrCl_6:Bi^{3+}	Bi	0.076	1.03	2.02	3	208.98	0.9638	0.4108	465	2.26
Cs_2ZrCl_6:Bi^{3+}	Bi	0.078	1.03	2.02	3	208.98	0.9636	0.4111	465	2.29

Table S2. *Cont.*

chemical_structure	D	D_conc	R	EN	V	M	t	μ	EW	τ
$Cs_2ZrCl_6:Bi^{3+}$	Bi	0.080	1.03	2.02	3	208.98	0.9633	0.4115	465	2.31
$Cs_2ZrCl_6:Bi^{3+}$	Bi	0.082	1.03	2.02	3	208.98	0.9631	0.4118	465	2.33
$Cs_2ZrCl_6:Bi^{3+}$	Bi	0.086	1.03	2.02	3	208.98	0.9626	0.4125	465	2.35
$Cs_2ZrCl_6:Bi^{3+}$	Bi	0.090	1.03	2.02	3	208.98	0.9622	0.4132	465	2.38
$Cs_2ZrCl_6:Bi^{3+}$	Bi	0.094	1.03	2.02	3	208.98	0.9617	0.4139	465	2.40
$Cs_2ZrCl_6:Bi^{3+}$	Bi	0.098	1.03	2.02	3	208.98	0.9612	0.4146	465	2.42
$Cs_2ZrCl_6:Bi^{3+}$	Bi	0.100	1.03	2.02	3	208.98	0.9610	0.4149	465	2.45
$Cs_2ZrCl_6:Bi^{3+}$	Bi	0.104	1.03	2.02	3	208.98	0.9605	0.4156	465	2.47
$Cs_2ZrCl_6:Bi^{3+}$	Bi	0.108	1.03	2.02	3	208.98	0.9601	0.4163	465	2.49
$Cs_2ZrCl_6:Bi^{3+}$	Bi	0.112	1.03	2.02	3	208.98	0.9596	0.4170	465	2.51
$Cs_2ZrCl_6:Bi^{3+}$	Bi	0.116	1.03	2.02	3	208.98	0.9591	0.4177	465	2.54
$Cs_2ZrCl_6:Bi^{3+}$	Bi	0.120	1.03	2.02	3	208.98	0.9587	0.4183	465	2.56

Table S3. Summary of models used in this work.

Models name	Description
sklearn.linear_model.Ridge	Linear regressor
sklearn.neighbors.KNeighborsRegressor	K-nearest neighbors regressor
sklearn.tree.DecisionTreeRegressor	Decision tree regressor
sklearn.neural_network.MLPRegressor	Multi-layer Perceptron regressor
sklearn.ensemble.RandomForestRegressor	Random Forest regressor
sklearn.svm.SVR	Support vector regressor
Xgboost.XGBRegressor	Extreme gradient boosting regressor

Table S4. Summary of optimized hyperparameters used in regression models.

Models	Parameters
RR for predicting EW	'alpha': 0.0003321278571510038, 'copy_X': True, 'fit_intercept': True, 'positive': False, 'solver': 'cholesky', 'tol': 0.0001
RR for predicting τ	'alpha': 1.2259340307824374e-05, 'copy_X': True, 'fit_intercept': False, 'positive': False, 'solver': 'auto', 'tol': 0.0001
KNR for predicting EW	'algorithm': 'auto', 'leaf_size': 30, 'metric': 'minkowski', 'metric_params': None, 'n_jobs': None, 'n_neighbors': 8, 'p': 1, 'weights': 'uniform'
KNR for predicting τ	'algorithm': 'auto', 'leaf_size': 30, 'metric': 'manhattan', 'metric_params': None, 'n_jobs': None, 'n_neighbors': 5, 'p': 2, 'weights': 'uniform'
SVR for predicting EW	'C': 9.757228091152033, 'cache_size': 200, 'coef0': 0.0, 'degree': 3, 'epsilon': 0.029103262337218397, 'gamma': 'scale', 'kernel': 'linear', 'max_iter': -1, 'shrinking': True, 'tol': 0.001, 'verbose': False
SVR for predicting τ	'C': 9.937494751747728, 'cache_size': 200, 'coef0': 0.0, 'degree': 3, 'epsilon': 0.040073794933765935, 'gamma': 'scale', 'kernel': 'linear', 'max_iter': -1, 'shrinking': True, 'tol': 0.001, 'verbose': False
MLPR for predicting EW	'activation': 'relu', 'alpha': 0.03760224927793436, 'batch_size': 'auto', 'beta_1': 0.9, 'beta_2': 0.999, 'early_stopping': False, 'epsilon': 1e-08, 'hidden_layer_sizes': (256, 128), 'learning_rate': 'constant', 'learning_rate_init': 0.001, 'max_fun': 15000, 'max_iter': 19000, 'momentum': 0.9, 'n_iter_no_change': 150, 'nesterovs_momentum': True, 'power_t': 0.5, 'random_state': None, 'shuffle': True, 'solver': 'adam', 'tol': 7.187333681105005e-05, 'validation_fraction': 0.1, 'verbose': False, 'warm_start': False

Table S4. *Cont.*

Models	Parameters
MLPR for predicting τ	'activation': 'relu', 'alpha': 0.35724177191478235, 'batch_size': 'auto', 'beta_1': 0.9, 'beta_2': 0.999, 'early_stopping': False, 'epsilon': 1e-08, 'hidden_layer_sizes': (256, 128), 'learning_rate': 'constant', 'learning_rate_init': 0.001, 'max_fun': 15000, 'max_iter': 12000, 'momentum': 0.9, 'n_iter_no_change': 200, 'nesterovs_momentum': True, 'power_t': 0.5, 'random_state': None, 'shuffle': True, 'solver': 'adam', 'tol': 4.6943183404648796e-05, 'validation_fraction': 0.1, 'verbose': False, 'warm_start': False
RFR for predicting EW	'bootstrap': True, 'ccp_alpha': 0.0, 'criterion': 'squared_error', 'max_depth': None, 'max_features': None, 'max_leaf_nodes': None, 'max_samples': None, 'min_impurity_decrease': 0.0, 'min_samples_leaf': 6, 'min_samples_split': 5, 'min_weight_fraction_leaf': 0.0, 'monotonic_cst': None, 'n_estimators': 250, 'n_jobs': None, 'oob_score': False, 'random_state': None, 'verbose': 0, 'warm_start': False
RFR for predicting τ	'bootstrap': False, 'ccp_alpha': 0.0, 'criterion': 'squared_error', 'max_depth': 5, 'max_features': 'sqrt', 'max_leaf_nodes': None, 'max_samples': None, 'min_impurity_decrease': 0.0, 'min_samples_leaf': 1, 'min_samples_split': 4, 'min_weight_fraction_leaf': 0.0, 'monotonic_cst': None, 'n_estimators': 650, 'n_jobs': None, 'oob_score': False, 'random_state': None, 'verbose': 0, 'warm_start': False
XGBR for predicting EW	'objective': 'reg:squarederror', 'base_score': None, 'booster': None, 'callbacks': None, 'colsample_bylevel': None, 'colsample_bynode': None, 'colsample_bytree': 1.0, 'device': None, 'early_stopping_rounds': None, 'enable_categorical': False, 'eval_metric': None, 'feature_types': None, 'feature_weights': None, 'gamma': 0.1, 'grow_policy': None, 'importance_type': None, 'interaction_constraints': None, 'learning_rate': 0.0241355159221002, 'max_bin': None, 'max_cat_threshold': None, 'max_cat_to_onehot': None, 'max_delta_step': None, 'max_depth': 3, 'max_leaves': None, 'min_child_weight': 3, 'missing': nan, 'monotone_constraints': None, 'multi_strategy': None, 'n_estimators': 200, 'n_jobs': None, 'num_parallel_tree': None, 'random_state': 42, 'reg_alpha': 0.5, 'reg_lambda': 1.5, 'sampling_method': None, 'scale_pos_weight': None, 'subsample': 0.6, 'tree_method': None, 'validate_parameters': None, 'verbosity': None
XGBR for predicting τ	'objective': 'reg:squarederror', 'base_score': None, 'booster': None, 'callbacks': None, 'colsample_bylevel': None, 'colsample_bynode': None, 'colsample_bytree': 0.6, 'device': None, 'early_stopping_rounds': None, 'enable_categorical': False, 'eval_metric': None, 'feature_types': None, 'feature_weights': None, 'gamma': 0.3, 'grow_policy': None, 'importance_type': None, 'interaction_constraints': None, 'learning_rate': 0.027437834976407963, 'max_bin': None, 'max_cat_threshold': None, 'max_cat_to_onehot': None, 'max_delta_step': None, 'max_depth': 3, 'max_leaves': None, 'min_child_weight': 1, 'missing': nan, 'monotone_constraints': None, 'multi_strategy': None, 'n_estimators': 400, 'n_jobs': None, 'num_parallel_tree': None, 'random_state': 42, 'reg_alpha': 0.30000000000000004, 'reg_lambda': 1.5, 'sampling_method': None, 'scale_pos_weight': None, 'subsample': 1.0, 'tree_method': None, 'validate_parameters': None, 'verbosity': None

Table S5. Quantitative overfitting evaluation for the prediction target EW.

Model	Train R^2	Test R^2	R^2 Gap	Train MSE	Test MSE	Assessment
RR	0.9969	0.9982	−0.0013	87.7635	44.6618	No obvious overfitting
KNR	0.9980	0.9999	−0.0019	56.6353	1.4434	No obvious overfitting
SVR	0.9900	0.9826	0.0075	285.7299	441.1791	No obvious overfitting
RFR	0.9980	0.9998	−0.0018	57.7345	5.9468	No obvious overfitting
XGBR	0.9982	0.9995	−0.0013	52.4383	13.1429	No obvious overfitting
MLPR	0.9978	0.9996	−0.0018	64.3239	10.0158	No obvious overfitting

R^2 gap > 0.15: Obvious overfitting with insufficient generalization capacity

$0.05 < R^2$ gap ≤ 0.15: Mild overfitting, generally acceptable

R^2 gap ≤ 0.05: Negligible overfitting with strong generalization ability

Table S6. Quantitative overfitting evaluation for the prediction target τ.

Model	Train R^2	Test R^2	R^2 Gap	Train MSE	Test MSE	Assessment
RR	0.9899	0.9771	0.0128	1.1370	1.9793	No obvious overfitting
KNR	0.9943	0.9851	0.0091	0.6488	1.2830	No obvious overfitting
SVR	0.9810	0.9578	0.0232	2.1472	3.6452	No obvious overfitting
RFR	0.9946	0.9887	0.0059	0.6075	0.9747	No obvious overfitting
XGBR	0.9948	0.9862	0.0086	0.5833	1.1924	No obvious overfitting
MLPR	0.9935	0.9875	0.0061	0.7293	1.0822	No obvious overfitting

R^2 gap > 0.15: Obvious overfitting with insufficient generalization capacity

$0.05 < R^2$ gap ≤ 0.15: Mild overfitting, generally acceptable

R^2 gap ≤ 0.05: Negligible overfitting with strong generalization ability

2. Partial code

The machine learning program was compiled and run using Jupyter Notebook.

```
## Feature Engineering
data=pd.read_excel('Supporting Information TABLE S2.xlsx')
data.head()
data.info()
data.isnull().sum()
data.columns
database1_name = ['D']
database1 = data[database1_name]
from sklearn.preprocessing import OneHotEncoder
onehot1 = OneHotEncoder()
A = onehot1.fit_transform(database1).toarray()
pd.DataFrame(A)
label = onehot1.categories_
col = list(label[0])
data1 = pd.DataFrame(A, columns=col)
```

```
data1
database2_name = [ 'D_conc', 'R', 'EN', 'Valence', 'M', 't', 'μ', 'EW', 'τ']
data2 = data[database2_name]
data3=pd.concat([data1,data2],axis=1)
data3
data3.columns
data3.columns
data4_columns = data3.columns.drop('μ')
data4=data3[data4_columns]
data4
plt.figure(figsize=(15,12),dpi=600)
corr=data4.corr()
mask = np.triu(np.ones_like(corr,dtype=bool))
sns.heatmap(corr,mask=mask,annot=True,cmap='coolwarm')
## Specify the feature matrix X and target variable Y, and split the dataset into training and test sets.
X = data4.iloc[:,0:12]
Y = data4.iloc[:,12:14]
print("Print the column names of X ", X.columns)
print("Print the column names of Y ", Y.columns)
from sklearn.model_selection import train_test_split
x_train,x_test,y_train,y_test=train_test_split(X,Y,test_size=0.2,random_state=42)
print("Training set input ", x_train.shape)
print("Training set output ", y_train.shape)
print("Test set input", x_test.shape)
print("Test set output ", y_test.shape)
print("Column names of the test set output ", y_train.columns)

## Hyperparameter Optimization for Multi-layer Perceptron Regressor
%%time
import optuna
from sklearn.metrics import mean_squared_error
from sklearn.model_selection import cross_val_score
def objective(trial, x_train, y_value):
    params = {
        "hidden_layer_sizes": trial.suggest_categorical('hidden_layer_sizes',
         [(32,), (64,), (64, 32), (128,), (128, 64), (128, 64, 32), (256,), (256, 128)]),
        "solver": trial.suggest_categorical('solver', ['adam', 'sgd']),
        "max_iter": trial.suggest_int('max_iter', 5000, 30000, step=1000),
        "alpha": trial.suggest_float('alpha', 1e-5, 1.0, log=True),
        "early_stopping": True,
        "n_iter_no_change": trial.suggest_int('n_iter_no_change', 50, 200, step=50),
        "tol": trial.suggest_float('tol', 1e-5, 1e-3, log=True)
    }
    model = MLPRegressor(**params)
    scores = cross_val_score(model, x_train, y_value, cv=10,
scoring='neg_root_mean_squared_error',n_jobs=-1,verbose=0)
    return scores.mean()

variables = {'EW': y_train['EW'],
    'τ': y_train['τ']
}
mlp_best_models = {}
```

```
for y_name, y_value in variables.items():
    print(f"Optimizing for {y_name}...")
    study = optuna.create_study(
        direction='maximize',
        sampler=optuna.samplers.CmaEsSampler(seed=42),
        pruner=optuna.pruners.SuccessiveHalvingPruner()
        )
    study.optimize(lambda trial: objective(trial, x_train, y_value), n_trials=50,
     timeout=600, show_progress_bar=True)
    best_params = study.best_params
    print(f"{y_name} Best Parameters:", best_params)
    print(f"{y_name} Best Score:", study.best_value)
    mlp_best_model = MLPRegressor(**best_params)
    mlp_best_models[y_name]=mlp_best_model
    print(f"{y_name} Best Model:", mlp_best_models[y_name])
print('=====================================================')

## Model Evaluation
models = [ridge_best_models, knn_best_models, svr_best_models, rf_best_models, xgb_best_models,
mlp_best_models]

y_columns = ['EW', 'τ']
for y_col in y_columns:
        print(f"  target variable: {y_col}")

        model_names = [model[y_col].__class__.__name__ for model in models]

        model[y_col].fit(x_train, y_train[y_col])
        y_predict_test1 = model[y_col].predict(x_test)


        r2 = r2_score(y_test[y_col], y_predict_test1)
        MAE = mean_absolute_error(y_test[y_col], y_predict_test1)
        MSE = mean_squared_error(y_test[y_col], y_predict_test1)

        print(f"{y_col}的{model[y_col].__class__.__name__} r2: {r2}")
        print(f"{y_col}的{model[y_col].__class__.__name__} MAE: {MAE}")
        print(f"{y_col}的{model[y_col].__class__.__name__} MSE: {MSE}")
        print("++++++++++++++++++++++++++")


## Model Explanation
import shap
import matplotlib.ticker as ticker

KNR = knn_best_models['EW']
KNR.fit(x_train, y_train)
explainer = shap.KernelExplainer(KNR.predict, x_train)
SHAP_value = explainer(x_train)
print("SHAP value:", SHAP_value.shape)
if len(SHAP_value.shape) > 2:
```

```
    SHAP_value = SHAP_value[:, :, 0]
    print("processed SHAP value:", SHAP_value.shape)
print("The shape of the test set data:", x_test.shape)
if len(x_test.shape) > 2:
    x_test = x_test.reshape(x_test.shape[0], -1)
    print("The shape of the processed test set data.:", x_test.shape)
assert SHAP_value.shape[1] == x_test.shape[1], " The number of features in the SHAP values does
not match the number of features in the input data. "

plt.figure(figsize=(6, 6), dpi=600)
shap.plots.beeswarm(SHAP_value,
    max_display=None,
    color_bar=True,
    show=False)
plt.gca().set_xscale('symlog', linthresh=1)
def format_func(x, pos):
    if x < 0:
        return f"-{abs(x):.2g}"
    else:
        return f"{x:.2g}"

plt.gca().xaxis.set_major_formatter(ticker.FuncFormatter(format_func))
plt.gca().spines['bottom'].set_linewidth(2)
plt.show()
```

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