PCCP

SUPPLEMENTARY MATERIAL

Trapping and thermal migration of the first- and second-row atoms in Ar, Kr and Xe crystals.

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I. *AB INITIO* CALCULATIONS OF THE DIATOMIC POTENTIALS

All ab initio calculations were performed in the MOLPRO programm package using the restricted version of the coupled cluster method with single, double and noniterative triple excitations (RCCSD(T)) along with and the correlation-consistent aug-cc-pV5Z basis sets for H-Ne atoms[73–76] with the addition of 3s3p2d2f1 bond function set placed at the midpoint of internuclear distance.

All guest atoms were taken in their respective ground states (doublet was assumed for H, Li, B, C and F, triplet for oxygen, peptet for nitrogen and singlet for the rest). For Ar, scalar relativistic X2C correction was employed and the specially optimized aug-cc-pV5Z-X2C basis set[77,78] was used. In case of Kr and Xe relativistic effects were to some degree incorporated via the effective core pseudopotentials[80] (ECP10MDF and ECP28MDF for Kr and Xe, respectively) and supplementary aug-cc-pV5Z-PP basis sets[79,80] were used for the representation of the outer electronic shells. In order to separate V_{Σ}, cm^{-1} and V_{Π}, cm^{-1} states of the diatomic the number of occupied molecular orbitals with certain angular momenta was enforced and ensured by orbital rotation when needed. Interaction energies were computed over a tight grid of interatomic distances from 1.8 to 25 Åand corrected for basis set superposition error using the full counterpoise correction scheme[82].

The calculated potentials were approximated by the piecewise-analytic dependence ($e^{-\alpha r}$ – cubic spline – Ar^{-6}), described in greater detail in Ref. 83. The raw data points used in the construction of the potentials are presented in tables below. Evident distance grid non-uniformity stems from the fact that different diatomic curves have their important features at different distances and in order to construct a realistic interpolation, additional data points were sometimes calculated and added.

Many-body interactions involving guest atoms were not accounted for, but a calculation on a model system showed that they constitute around 5% of the total interaction energy. Due to the same sign of the many-body contributions to interaction energy, they are expected to have negligible effect on stability diagrams and trapping site structures, but may influence TIM barriers and their impact is one of the possible reasons for TIM barrier overestimation.

TABLE S.1: Results of CCSD(T) calculation for H–RG diatomics

	Ar	Kr	Xe
R, Å	Energy, cm^{-1}		
25	-0.000391188	-0.00054505	-0.000844143
22	-0.000826265	-0.001206387	-0.00182684
20	-0.001492966	-0.002148052	-0.003246087
17	-0.003988927	-0.005745766	-0.008673186
15	-0.008506124	-0.012260133	-0.018524738
12	-0.032941606	-0.047568165	-0.072136938
10	-0.100338917	-0.145199297	-0.221194591
9	-0.191782744	-0.278137113	-0.425488604
8	-0.398270033	-0.57927463	-0.891041271
7	-0.921130573	-1.345800148	-2.087908087
6	-2.463840187	-3.617898786	-5.669992864
5.5	-4.301594292	-6.330899641	-9.933126992
5.3	-5.445364577	-8.012474458	-12.5483975
5.2	-6.142462053	-9.033020897	-14.12252506
5.1	-6.93951744	-10.19536362	-15.90183232
5	-7.850500088	-11.51762812	-17.90722528
4.9	-8.890531557	-13.01890844	-20.15845922
4.8	-10.07582997	-14.7184643	-22.67235746
4.7	-11.42306231	-16.63450784	-25.45996479
4.6	-12.94865461	-18.78231931	-28.52233995
4.5	-14.66703249	-21.17116022	-31.84744602
4.4	-16.5876091	-23.79989683	-35.38579993
4.3	-18.71134935	-26.6506161	-39.07055394
4.2	-21.0251071	-29.67967114	-42.76074227
4.1	-23.4940859	-32.80520668	-46.27713877
4	-26.05030452	-35.88974565	-49.32207134
3.9	-28.5768042	-38.71612857	-51.44373183
3.8	-30.88502579	-40.95451434	-52.03856177
3.7	-32.68264122	-42.11817246	-50.25004496
3.6	-33.52778699	-41.50564361	-44.90498423
3.5	-32.76721433	-38.12624313	-34.42724125
3.4	-29.45681909	-30.60474778	-16.73546699
3.3	-22.26484592	-17.05903941	10.88702306
3.2	-9.348459458	5.05826298	51.96576507
3.1	11.81743923	39.16316417	111.050103
3	44.67435057	89.79216084	193.9517064
2.9	93.88104379	162.9012384	307.9975335
2.8	165.6781138	266.2176146	462.309248
2.7	268.3198097	409.6645981	668.164843
2.6	412.5843839	605.8941299	939.5321393
2.5	612.4172252	870.9860376	1294.138581

2.4	885.8103156	1225.370975	1754.763623
2.3	1255.88368	1695.002434	2351.043036
2.2	1752.07687	2312.97679	3122.458951
2.1	2411.670839	3122.082122	4123.56947
2	3281.990473	4178.663875	5431.265276
1.9	4423.699262	5557.926553	7154.891464
1.8	5915.225598	7361.644151	9451.612163

TABLE S.2: Results of CCSD(T) calculation for He–RG diatomics

	Ar	Kr	Xe
R, Å		Energy, cm^{-1}	
25	-0.000211688	-0.000210914	-0.000389329
22	-0.000395579	-0.000515221	-0.000836333
20	-0.000696942	-0.000956573	-0.001483422
17	-0.001915592	-0.002636799	-0.003952485
15	-0.004064205	-0.005677636	-0.008428051
12	-0.015765228	-0.022114218	-0.032706651
10	-0.047745907	-0.067340822	-0.099884753
9	-0.090925911	-0.128550241	-0.191404456
8	-0.187868572	-0.266455465	-0.398651402
7	-0.429905359	-0.612397171	-0.924137626
6	-1.134660463	-1.62526848	-2.480795496
5.5	-1.971406603	-2.836088554	-4.339302409
5.3	-2.496284537	-3.594633686	-5.489569422
5.2	-2.818736319	-4.058982013	-6.185973
5.1	-3.190149613	-4.591865783	-6.976546131
5	-3.618635388	-5.203573012	-7.871428692
4.9	-4.113566106	-5.905479604	-8.879865355
4.8	-4.685564316	-6.709848001	-10.00898262
4.7	-5.346587217	-7.629357471	-11.26174384
4.6	-6.109743213	-8.676305624	-12.6338142
4.5	-6.98951154	-9.861213231	-14.10870735
4.4	-8.000688338	-11.1905169	-15.65054801
4.3	-9.157282633	-12.66295131	-17.19328179
4.2	-10.47027108	-14.26364438	-18.62530787
4.1	-11.94369033	-15.95534419	-19.7669507
4	-13.56852375	-17.6644484	-20.33817565
3.9	-15.3123613	-19.26016133	-19.90223018
3.8	-17.10493196	-20.52342675	-17.83931462
3.7	-18.81276584	-21.1015339	-13.19264062
3.6	-20.20271681	-20.44212189	-4.585466916
3.5	-20.88756755	-17.69712467	10.01234423
3.4	-20.24622173	-11.58272804	33.48004057
3.3	-17.30636744	-0.17593857	69.9419709

3.2	-10.56542498	19.37892921	125.2616513
3.1	2.27794507	51.2905574	207.741515
3	24.71928363	101.7184021	329.069709
2.9	62.02044516	179.6159059	505.5975351
2.8	122.0335399	297.9144868	760.0620082
2.7	216.3904555	475.1815544	1123.896623
2.6	362.2146291	737.9335249	1640.327334
2.5	584.567922	1123.844842	2368.481701
2.4	919.9182281	1686.169129	3388.753706
2.3	1421.019002	2499.774548	4809.73175
2.2	2163.759441	3669.30046	6776.977773
2.1	3256.676942	5340.037166	9483.798112
2	4853.919615	7712.164006	13184.19755
1.9	7172.654365	11059.00776	18208.25847
1.8	10516.07669	15750.08998	24979.91515

TABLE S.3: Results of CCSD(T) calculation for Li–RG diatomics

	Ar	Kr	Xe
R, Å	Energy, cm^{-1}		
25	-0.003464798	-0.005132922	-0.008233356
22	-0.007505948	-0.01124188	-0.017886856
20	-0.01341386	-0.020111059	-0.031940707
17	-0.036331151	-0.054318124	-0.086199322
15	-0.078218998	-0.117160911	-0.185992727
12	-0.3120122	-0.467875429	-0.744793505
10	-0.987459866	-1.485210963	-2.375555517
9	-1.94736423	-2.934971459	-4.708955109
8	-4.184419433	-6.317702122	-10.15520391
7.8	-4.926376366	-7.440784123	-11.95635155
7.6	-5.817492529	-8.790185092	-14.11923201
7.4	-6.888342266	-10.41239526	-16.71175439
7.2	-8.175047311	-12.36176902	-19.82026691
7	-9.71922202	-14.70079724	-23.53452667
6.9	-10.60228503	-16.0380152	-25.65093944
6.8	-11.5677402	-17.49925315	-27.95762663
6.7	-12.62152661	-19.09380229	-30.46732087
6.6	-13.76991118	-20.83068319	-33.19200982
6.5	-15.01836841	-22.71826421	-36.14194028
6.4	-16.371274	-24.76373566	-39.32496443
6.3	-17.83176434	-26.97242283	-42.74575943
6.2	-19.4005533	-29.34725081	-46.40500926
6.1	-21.07629046	-31.88800455	-50.29858705
6	-22.85381104	-34.59058394	-54.41635378
5.9	-24.72390196	-37.44637632	-58.74054898

5.8	-26.67283812	-40.44078115	-63.24362479
5.7	-28.68007168	-43.55170122	-67.8853769
5.6	-30.71815051	-46.7468122	-72.60939335
5.5	-32.7505292	-49.98057161	-77.34010089
5.4	-34.72935691	-53.18987266	-81.97654008
5.3	-36.5940362	-56.29065276	-86.3882954
5.2	-38.26711937	-59.1735714	-90.40831805
5.1	-39.64959027	-61.69983079	-93.82660359
5	-40.61276686	-63.69564535	-96.38346979
4.9	-40.98613472	-64.94521722	-97.7640507
4.8	-40.54356524	-65.18377251	-97.59667473
4.7	-38.99277018	-64.09299472	-95.45471221
4.6	-35.97709884	-61.30191232	-90.86128224
4.5	-31.09880717	-56.39179145	-83.29063278
4.4	-23.94097109	-48.89747575	-72.16189301
4.3	-14.07028516	-38.29634929	-56.82645946
4.2	-1.003626038	-23.99115073	-36.56548389
4.1	15.83222685	-5.300299668	-10.60922916
4	37.11207606	18.5297336	21.82372877
3.8	96.02508101	84.70412307	109.113661
3.6	181.8683225	180.1150398	231.3597217
3.4	300.2507035	309.3012046	395.2064824
3.2	454.6895912	475.8086574	609.6324106
3	645.7581059	684.106935	899.46592
2.8	874.9075312	950.7778393	1335.984376
2.6	1160.405492	1339.661831	2100.840683
2.4	1581.720767	2038.724496	3606.853623
2.2	2385.451275	3509.568877	6720.971608
2	4217.468719	6804.095903	13195.32009
1.8	8614.899898	14193.94982	26438.74687

TABLE S.4: Results of CCSD(T) calculation for Be–RG diatomics

	Ar	Kr	Xe
R, Å	Energy, cm^{-1}		
25	-0.001816011	-0.002764313	-0.004344833
22	-0.003867364	-0.006046243	-0.009414154
20	-0.007059468	-0.010807901	-0.016774324
17	-0.01949471	-0.029065347	-0.045039768
15	-0.042350396	-0.062370457	-0.096694794
12	-0.166659752	-0.24546986	-0.381702618
10	-0.517445318	-0.762629747	-1.191556626
9	-1.00321187	-1.482292438	-2.32560734
8	-2.125407848	-3.150316698	-4.968904864
7	-5.057732339	-7.51965817	-11.93611471

6.5	-8.230912346	-12.22838825	-19.43344306
6	-13.83354448	-20.5002901	-32.47763709
5.9	-15.38855083	-22.79498308	-36.05981601
5.8	-17.12905779	-25.36236911	-40.04503727
5.7	-19.07582905	-28.23029868	-44.46699956
5.6	-21.25071882	-31.42599452	-49.35636273
5.5	-23.71528998	-34.97465039	-54.73631974
5.4	-26.37254606	-38.8976245	-60.619149
5.3	-29.35626951	-43.21036015	-67.00043679
5.2	-32.63748973	-47.91856935	-73.85254205
5.1	-36.21573987	-53.01258689	-81.116346
5	-40.07746534	-58.45951515	-88.6901308
4.9	-44.1887863	-64.19258308	-96.41285606
4.8	-48.4865769	-70.09755806	-104.0400915
4.7	-52.86280887	-75.99455796	-111.2129163
4.6	-57.15004389	-81.61505821	-117.4218351
4.5	-61.09757316	-86.57275966	-121.9560837
4.4	-64.34858756	-90.32757541	-123.9054812
4.3	-66.40676914	-92.14327839	-122.0043169
4.2	-66.59568435	-91.03739665	-114.6609504
4.1	-64.00792275	-85.72033477	-99.81935757
4.05	-61.3086023	-80.97582986	-88.78990693
4	-57.43270654	-74.51149514	-74.84279051
3.95	-52.16527941	-66.0352528	-57.52996371
3.9	-45.25897627	-55.21198344	-36.3460178
3.85	-36.42957356	-41.65773296	-10.68745759
3.8	-25.35245388	-24.9346726	19.96289981
3.75	-11.65909345	-4.547263426	56.41067049
3.7	5.067003198	20.06014796	99.37949697
3.6	49.55082286	84.46803737	208.2764928
3.5	112.5686322	174.004136	354.2262555
3.4	199.6721615	295.5059144	546.2204495
3.2	474.705501	668.5647151	1113.353636
3	947.047944	1289.545878	2022.121199
2.8	1717.218363	2275.261648	3423.548646
2.6	2911.590072	3768.304735	5518.155779
2.4	4668.571305	5943.649527	8621.877334
2.2	7141.234483	9064.772931	13343.71407
2	10598.96988	13750.88436	21151.71565
1.8	15933.69144	21818.15764	35578.97788

TABLE S.5: Results of CCSD(T) calculation for B–RG diatomics

	Ar		Kr		Xe	
R, Å	V_Π, cm^{-1}	V_Σ, cm^{-1}	V_Π, cm^{-1}	V_Σ, cm^{-1}	V_Π, cm^{-1}	V_Σ, cm^{-1}
25	-0.001339415	-0.00142158	-0.001980528	-0.002146093	-0.003065626	-0.003338931
22	-0.002883481	-0.003198692	-0.004341128	-0.004732902	-0.006654557	-0.007275984
20	-0.005289368	-0.005764392	-0.007751619	-0.008488932	-0.011848598	-0.013005294
17	-0.014255395	-0.015690399	-0.020797746	-0.022964536	-0.031721396	-0.035116455
15	-0.030544403	-0.033837859	-0.044451402	-0.049590724	-0.067901591	-0.075813224
12	-0.118712962	-0.134355429	-0.17296242	-0.196977109	-0.264688047	-0.302372386
10	-0.362748504	-0.421960941	-0.52939185	-0.620871158	-0.814538691	-0.958172227
9	-0.69448609	-0.828940102	-1.016490157	-1.220249998	-1.569367291	-1.892289268
8	-1.445250609	-1.785803741	-2.123059012	-2.634885368	-3.295470022	-4.112463779
7	-3.362700135	-4.333611774	-4.956826078	-6.417460321	-7.75959112	-10.07719095
6	-9.043079234	-12.05243174	-13.37973626	-17.81368983	-21.23295619	-27.87181234
5.5	-15.81204533	-20.72955176	-23.51870391	-30.50049142	-37.48339757	-46.95320676
5.3	-20.04250539	-25.70777134	-29.83223866	-37.61982737	-47.55783396	-57.20795415
5.1	-25.58569658	-31.65096596	-38.05504855	-45.92906015	-60.59396646	-68.62931363
5	-28.96984031	-34.94608662	-43.04980245	-50.43051957	-68.45541743	-74.49085891
4.8	-37.22633894	-41.88679494	-55.18242228	-59.59502118	-87.34912766	-85.30524648
4.6	-47.83831915	-48.38482806	-70.68025022	-67.46028764	-111.0419738	-91.86221795
4.5	-54.17724068	-50.87143034	-79.85338866	-69.91655913	-124.8271134	-91.68954719
4.45	-57.62864179	-51.75892483	-84.81234628	-70.50358515	-132.1917927	-90.24198298
4.4	-61.27611523	-52.32066463	-90.01914879	-70.52089401	-139.8827204	-87.66395434
4.35	-65.11753727	-52.47397093	-95.4686143	-69.83850755	-147.8492542	-83.70100922
4.3	-69.15303828	-52.12030388	-101.1509558	-68.30423374	-156.0707031	-78.10315008
4.25	-73.37363766	-51.14302265	-107.0482754	-65.74048473	-164.505208	-70.57052893
4.2	-77.76738923	-49.40483826	-113.1376758	-61.94049983	-173.0980149	-60.75864278
4.15	-82.31584386	-46.74424457	-119.3853809	-56.66420413	-181.7797647	-48.27294429
4.1	-86.99285966	-42.97324482	-125.7471152	-49.63351439	-190.4647916	-32.66312083
4.05	-91.763364	-37.87162132	-132.1657292	-40.52707464	-199.0491684	-13.41680406
4	-96.58207413	-31.18420071	-138.5689215	-28.97434438	-207.4085795	10.04746217
3.95	-101.3900776	-22.61434487	-144.8666518	-14.54894774	-215.3957468	38.38801583
3.9	-106.1150072	-11.81874401	-150.9483239	3.238774232	-222.8369907	72.34918974
3.85	-110.6668515	1.598878007	-156.6791852	24.95012585	-229.528202	112.7717861
3.8	-114.9354941	18.09508921	-161.8969323	51.22746052	-235.2293632	160.6055402
3.75	-118.7881701	38.19553208	-166.4072194	82.80444735	-239.6578112	216.9228054
3.7	-122.0652991	62.50349648	-169.9788778	120.5180785	-242.4806068	282.9357903
3.65		91.71144912				
3.6	-126.0875206	126.6154129	-173.1635607	218.2999539	-241.6690039	449.7023338
3.55		168.1292067				
3.5	-124.9603482	217.3020214	-168.631396	353.8797346	-228.7671261	674.1038751
3.4	-115.7670039	343.6080011	-152.5089599	539.2682793	-198.3560251	972.8200036
3.35	-106.9268739		-138.5211807	655.3116264	-174.4559706	1156.364168
3.3	-94.43779913	517.3649091	-119.5331603	789.9146162	-143.4073229	1366.63553

3.25	-77.56140197		-94.60952679	945.6863012	-104.04446	1606.980384
3.2	-55.44611919	753.9228039	-62.68105141	1125.564085	-55.0587381	1881.096688
3.15	-27.11438397		-22.53046399	1332.848819	5.029469778	2193.072297
3.1	8.553745684	1073.050541	27.22296272	1571.244475	77.90524292	2547.428324
3.05	52.83887124		88.14481424	1844.901245	165.4953834	2949.157075
3	107.2043471	1500.085504	162.0076792	2158.463143	270.0036741	3403.755017
2.95	173.3175797		250.8125965	2517.11638	393.9434011	3917.242643
2.9	253.0743094	2067.393102	356.8141571	2926.638935	540.166919	4496.169362
2.85	348.6200168		482.5436343	3393.446296	711.8938598	5147.597965
2.8	462.3718774	2816.098573	630.8331558	3924.638337	912.7407252	5879.067732
2.75	597.0383361		804.8410657	4528.036282	1146.762058	6698.536193
2.7	755.6363894	3797.975591	1008.079144	5212.217084	1418.515034	7614.304865
2.65	941.5042807		1244.443645	5986.535177	1733.162697	8634.931814
2.6	1158.308904	5077.315145	1518.253745	6861.131295	2096.624751	9769.128402
2.55	1410.052323		1834.302821	7846.925161	2515.781963	11025.62857
2.5	1701.081646	6732.454849	2197.929485	8955.58448	2998.734732	12413.0129
2.45	2036.114297		2615.1127	10199.46037	3555.114407	13939.46187
2.4	2420.279437	8856.74421	3092.590336	11591.46004	4196.441792	15612.41976
2.35	2859.167725		3638.003513	13144.82746	4936.530842	17438.15175
2.3	3358.878035	11558.55253	4260.076973	14872.78998	5791.918952	19421.22634
2.25	3926.0599		4968.861413	16788.03433	6782.418222	21564.10821
2.2	4567.973698	14958.03913	5776.071067	18901.94907	7931.928029	23867.25225
2.15	5292.598465		6695.564213	21223.54955	9269.728231	26330.38292
2.1	6108.831277	19176.09529	7744.022853	23757.96168	10832.22269	28955.34095
2.05	7026.834159		8941.932205		12664.89192	31750.24294
2	8058.619575	24307.47936	10314.97686	34601.66197	14824.40607	34734.59069
1.95	9219.000348					
1.9	10527.01795	30355.31249	13726.55386	46266.40256	20422.66203	41455.1691
1.85	12007.90799					
1.8	13695.61373	51808.3082	18368.65891	61863.50262	28420.6344	49949.37433

TABLE S.6: Results of CCSD(T) calculation for C–RG diatomics

	Ar		Kr		Xe	
R, Å	V_Π, cm^{-1}	V_Σ, cm^{-1}	V_Π, cm^{-1}	V_Σ, cm^{-1}	V_Π, cm^{-1}	V_Σ, cm^{-1}
25	-0.001027548	-0.000972505	-0.001468077	-0.00138565	-0.002282851	-0.002154551
22	-0.002261892	-0.00210919	-0.00325361	-0.003070329	-0.00495855	-0.004673954
20	-0.004084141	-0.003869909	-0.005827693	-0.00549478	-0.008833474	-0.008316431
17	-0.010905224	-0.010214944	-0.015717296	-0.014758502	-0.023724667	-0.022231178
15	-0.02326656	-0.021862346	-0.033637338	-0.031526027	-0.050791946	-0.047482445
12	-0.091084776	-0.084999884	-0.131379328	-0.122405416	-0.198976812	-0.184880919
10	-0.279997513	-0.258994941	-0.405996164	-0.373255891	-0.617302437	-0.566917349
9	-0.540087246	-0.493429518	-0.783848934	-0.71447737	-1.197137201	-1.089014539
8	-1.134336694	-1.020986956	-1.650620351	-1.48494296	-2.535910467	-2.274914987
7	-2.667556127	-2.358352329	-3.89721716	-3.43906693	-6.038618827	-5.323309054

6	-7.2948476	-6.304987212	-10.68013093	-9.228810396	-16.6776865	-14.51810223
5.5	-12.80475932	-10.99811447	-18.79258956	-16.26323015	-29.24096124	-25.85749162
5.3	-16.21228919	-13.96556039	-23.76238508	-20.72742475	-36.78476075	-33.10125595
5.1	-20.61474765	-17.91307147	-30.10542998	-26.66496334	-46.20032367	-42.75701396
5	-23.26166258	-20.36193374	-33.87592412	-30.34952293	-51.66847545	-48.75312859
4.8	-29.58250157	-26.49810653	-42.73553749	-39.58036062	-64.0815688	-63.77756672
4.6	-37.37331755	-34.79484422	-53.31746989	-52.03572938	-77.91418274	-84.0323971
4.5	-41.79215768	-39.98956149	-59.1072419	-59.81237737	-84.8627857	-96.65600036
4.45	-44.10843653	-42.89778595	-62.06488846	-64.1576805	-88.1832222	-103.7001746
4.4	-46.47831769	-46.03431882	-65.04856042	-68.83696296	-91.29944349	-111.2677418
4.35	-48.88258976	-49.41595747	-67.94840446	-73.87330743	-94.15277495	-119.4238257
4.3	-51.29636872	-53.06011248	-70.78568671	-79.29053742	-96.60675241	-128.1748851
4.25	-53.68744915	-56.98494632	-73.47489173	-85.11293394	-98.54292851	-137.5677592
4.2	-56.01493538	-61.20848245	-75.94076229	-91.36494448	-99.80773172	-147.6396647
4.15	-58.22734097	-65.74897056	-78.09040136	-98.07074806	-100.2182623	-158.42769
4.1	-60.26023819	-70.62413906	-79.81154416	-105.2536745	-99.55777116	-169.9683265
4.05	-62.03401058	-75.8502755	-80.96761577	-112.9354835	-97.5703638	-182.2967267
4	-63.45060276	-81.44232848	-81.39418245	-121.1355257	-93.95522737	-195.4459643
3.95	-64.39033244	-87.41230356	-80.89389089	-129.8696624	-88.35905623	-209.4461882
3.9	-64.70764593	-93.76924882	-79.2309126	-139.1492074	-80.36948159	-224.3235847
3.85	-64.22663589	-100.5171265	-76.12460784	-148.9796523	-69.50559197	-240.0991131
3.8	-62.73548892	-107.6542287	-71.24230789	-159.3591007	-55.20869517	-256.7878996
3.75	-59.97946811	-115.1713171	-64.19058671	-170.2766898	-36.8310251	-274.3980858
3.7	-55.65635161	-123.0498902	-54.50633024	-181.7103302	-13.62384973	-292.9283051
3.6	-40.79391204	-139.7564003	-24.96986608	-205.9668173	50.86655359	-332.6879625
3.5	-14.37301011	-157.3438771	22.93601852	-231.6208021	146.8739793	-375.7732758
3.4	28.86124877	-175.0487066	96.80275525	-257.7635777	285.8013183	-421.4872652
3.35	58.95561763	-183.5779643	146.5584466	-270.5791838	375.8879882	-444.945821
3.3	96.1693584	-191.6145229	206.9181553	-282.8938108	482.6725796	-468.4990219
3.25	141.8433694	-198.8824344	279.7352018	-294.3825691	608.7555298	-491.8405026
3.2	197.5491773	-205.0359339	367.1544519	-304.6448469	757.086085	-514.5950586
3.15	265.1264114	-209.6479913	471.6527652	-313.1941901	930.9937286	-536.3133481
3.1	346.7220268	-212.196251	596.0820593	-319.4458471	1134.221004	-556.4643691
3.05	444.8351082	-212.049856	743.716756	-322.7039013	1370.961289	-574.4203992
3	562.3663753	-208.4554537	918.3074365	-322.1454377	1645.905413	-589.4277668
2.95	702.6714919	-200.5232592	1124.140939	-316.8005979	1964.297648	-600.5607138
2.9	869.6250265	-187.2063635	1366.108148	-305.5269436	2331.996195	-606.6606394
2.85	1067.692485	-167.2769533	1649.781579	-286.976364	2755.529845	-606.2643041
2.8	1302.017311	-139.2939546	1981.499559	-259.5559532	3242.143124	-597.527127
2.75	1578.516412	-101.5652027	2368.456244	-221.3800347	3799.824326	-578.1366541
2.7	1903.987433	-52.10622876	2818.790662	-170.2204517	4437.311553	-545.2133781
2.65	2286.219782	11.40168422	3341.674873	-103.4494381	5164.072997	-495.1964147
2.6	2734.11121	91.65478547	3947.397946	-17.96902045	5990.260888	-423.7013423
2.55	3257.790959	191.7745171	4647.446586	89.87209092	6926.647773	-325.3314967
2.5	3868.743461	315.3619225	5454.57984	224.3931604	7984.560139	-193.4152254
2.45	4579.933137	466.5592445	6382.893755	390.7171534	9175.821515	-19.64556236

2.4	5405.922289	650.1205768	7447.871551	594.951808	10512.6977	206.380932
2.35	6362.972798	871.4968436	8666.410557	844.415775	12007.81414	497.7041527
2.3	7469.126442	1136.936654	10056.80853	1147.91822	13674.03124	870.5959348
2.25	8744.241342	1453.613352	11638.67975	1516.093405	15524.24763	1345.20026
2.2	10209.99246	1829.792008	13432.7635	1961.794825	17571.30753	1946.273401
2.15	11889.77836	2275.037576	15460.58636	2500.562134	19828.01258	2704.033464
2.1	13808.48359	2800.469778	17743.93726	3151.189957	22307.7449	3655.357196
2.05	15992.03653	3419.061852	20304.10809	3936.444842	25026.10808	4845.402898
2	18466.64475	4146.011289	23160.86629	4884.010374	28004.38993	6330.035018
1.95	21257.61153	4999.236189	26331.16864	6027.788567	31274.96693	8178.860261
1.9	24387.59051	6000.097311	29827.75178	7409.699903	34888.50538	10479.00893
1.85	27874.059	7174.456648	33658.04555	9082.129763	38922.73346	13339.72333
1.8	31725.78041	8554.207595	37824.76185	11111.22112	43493.77779	16898.13897

TABLE S.7: Results of CCSD(T) calculation for N–RG diatomics

	Ar	Kr	Xe
R, Å	Energy, cm^{-1}		
25	-0.000694497	-0.001036543	-0.001624871
22	-0.001650284	-0.002321102	-0.003530894
20	-0.002920085	-0.004166206	-0.00628252
17	-0.007862079	-0.011220821	-0.016793412
15	-0.016867355	-0.024006718	-0.035861965
12	-0.065515504	-0.093400152	-0.139842274
10	-0.19978228	-0.285679553	-0.429765794
9	-0.382372313	-0.547886497	-0.827630142
8	-0.794909643	-1.142254726	-1.735269256
7	-1.842783354	-2.657490255	-4.071548699
6	-4.956824381	-7.168599822	-11.11443498
5.5	-8.674610003	-12.61458625	-19.61093443
5.3	-11.00964702	-16.02777285	-24.88837294
5.2	-12.44270376	-18.11253746	-28.08528737
5.1	-14.08965115	-20.49847825	-31.71433051
5	-15.98149123	-23.22680385	-35.82050154
4.9	-18.15231215	-26.34141451	-40.44595282
4.8	-20.63999523	-29.88759218	-45.62635847
4.7	-23.48635704	-33.90937737	-51.38428318
4.6	-26.7361116	-38.44502086	-57.71702075
4.5	-30.43165509	-43.51907267	-64.57697976
4.4	-34.60494324	-49.13019303	-71.84470654
4.3	-39.26738129	-55.2335379	-79.28311386
4.2	-44.3959214	-61.71422911	-86.53966886
4.1	-49.91213261	-68.35024588	-92.98252766
4	-55.64989012	-74.75862061	-97.71138176
3.9	-61.30770829	-80.31936089	-99.38394919

3.8	-66.37879298	-84.06844835	-96.04969509
3.75	-68.455313	-84.83241378	-91.67096712
3.7	-70.0478065	-84.54727631	-84.90675137
3.65	-70.98153505	-82.91886589	-75.22139542
3.6	-71.04061145	-79.59137685	-61.98119842
3.55	-69.96055782	-74.13595937	-44.44024814
3.5	-67.41809657	-66.03738438	-21.72371977
3.45	-63.02109854	-54.6786837	7.191007855
3.4	-56.29508717	-39.32322217	43.49655406
3.35	-46.6673951	-19.09393447	88.58203886
3.3	-33.44832816	7.050993367	144.0643278
3.25	-15.80878678	40.34649384	211.8234227
3.2	7.246499842	82.25366008	294.0434715
3.15	36.91079133	134.4978671	393.2542201
3.1	74.61010383	199.1122048	512.376231
3	181.2466098	375.4232093	824.2903321
2.9	345.0016146	635.6308816	1262.861742
2.8	590.8900264	1012.949391	1870.693504
2.7	953.6126383	1552.043002	2701.82554
2.6	1480.835903	2312.40517	3824.086673
2.5	2237.516196	3372.518888	5321.408673
2.4	3311.360513	4834.498492	7295.030105
2.2	6913.319471	9517.884875	13163.09963
2	13684.16611	17811.71458	22636.25806
1.8	24868.96258	30711.77260	61452.36640

TABLE S.8: Results of CCSD(T) calculation for F–RG diatomics

	Ar		Kr		Xe	
R, Å	V_{Π}, cm^{-1}	V_{Σ}, cm^{-1}	V_{Π}, cm^{-1}	V_{Σ}, cm^{-1}	V_{Π}, cm^{-1}	V_{Σ}, cm^{-1}
25	-0.000506488	-0.000467614	-0.000633254	-0.000611521	-0.00101733	-0.000978082
22	-0.001132169	-0.001050054	-0.001440792	-0.001392936	-0.002194948	-0.002118958
20	-0.001925997	-0.001812518	-0.002597376	-0.002510982	-0.003899401	-0.003766198
17	-0.005062734	-0.004901399	-0.007028204	-0.006788608	-0.010422215	-0.010057663
15	-0.010735629	-0.010397314	-0.015060277	-0.014529399	-0.02226964	-0.02146154
12	-0.04170448	-0.040145592	-0.058640276	-0.0563958	-0.086776235	-0.083347666
10	-0.126940928	-0.121867963	-0.179385652	-0.171662166	-0.266551977	-0.25502494
9	-0.243052933	-0.231813286	-0.344022621	-0.328060377	-0.513466285	-0.489194035
8	-0.505655568	-0.488759719	-0.717432275	-0.680414424	-1.077111784	-1.019543357
7	-1.17155302	-1.101505747	-1.668750645	-1.570044696	-2.527030198	-2.375188395
6	-3.145167321	-2.927006056	-4.500337384	-4.189854317	-6.898213579	-6.439115845
5.5	-5.51588131	-5.100392781	-7.931082917	-7.361069652	-12.19082	-11.43297421
5.3	-7.009335908	-6.470946179	-10.09243929	-9.376114965	-15.48966129	-14.62982535
5.2	-7.928619056	-7.317600187	-11.41759491	-10.62200404	-17.49327764	-16.61176149
5.1	-8.988765751	-8.297700145	-12.93901745	-12.06439159	-19.77202631	-18.90916593

5	-10.21225356	-9.435190968	-14.68520986	-13.73801172	-22.35566423	-21.57651025
4.9	-11.62414074	-10.75751034	-16.68693278	-15.68387643	-25.27095168	-24.67755704
4.8	-13.25165105	-12.29720465	-18.97598028	-17.94989228	-28.53821247	-28.28669502
4.7	-15.12435899	-14.09273496	-21.58430064	-20.59207281	-32.16539321	-32.49060357
4.6	-17.27406132	-16.1903112	-24.53913878	-23.67622914	-36.14073599	-37.39011222
4.5	-19.73441263	-18.64687963	-27.86037521	-27.27817881	-40.41735996	-43.10104307
4.4	-22.53732037	-21.52983163	-31.55098721	-31.48515876	-44.89382704	-49.75478445
4.3	-25.70579936	-24.91652214	-35.58582411	-36.39597988	-49.38466405	-57.49646107
4.2	-29.24265347	-28.89211292	-39.89166	-42.11924308	-53.5659471	-66.47256908
4.1	-33.11424941	-33.5469743	-44.3171525	-48.7686331	-56.96375378	-76.87666952
4	-37.22763803	-38.97348754	-48.58734403	-56.45379226	-58.76808729	-88.84328172
3.9	-41.3952323	-45.25997098	-52.24194778	-65.26712765	-57.81365124	-102.5430125
3.8	-45.28354883	-52.47905567	-54.52371359	-75.26541054	-52.36355647	-118.1241307
3.7	-48.33045871	-60.66602493	-54.28514733	-86.44307334	-39.88629007	-135.7114716
3.6	-49.62323889	-69.78080189	-49.75979031	-98.69546345	-16.72561425	-155.3895125
3.5	-47.71724279	-79.65058399	-38.30689869	-111.7503256	22.36399643	-177.1692606
3.4	-40.38088833	-89.89141883	-28.82273578	-118.427231	84.86140637	-200.9609775
3.35	-33.67616684	-94.9452971	-16.00940426	-125.0765779	128.0442342	
3.3	-24.22588792	-99.78864003	0.916170202	-131.5651065	181.3473783	-226.5666055
3.25	-11.3355339	-104.2487227	22.90192007	-137.7260697	246.7642231	
3.2	5.844253753	-108.102578	51.09232331	-143.3413473	326.6428576	-253.7541958
3.15	28.34956942	-111.0656051	86.86598585	-148.139762	423.7424657	
3.1	57.4416152	-112.7787445	131.8792346	-151.7863579	541.2995123	-282.4490814
3.05	94.6521321	-112.7929431	188.1173606	-153.8721424	683.106461	
3	141.8371419	-110.5509211	257.955177	-153.9020703	853.6039786	-312.9860382
2.95	201.2420374	-105.3647535	344.2288639	-151.280387	1057.984045	-329.2079167
2.9	275.5801506	-96.38808968	450.3212361	-145.1619841	1302.305494	-346.2907696
2.85	368.1269382	-82.58191414	580.2627853	-135.101895		-364.4514954
2.8	482.8325575	-62.67393567	931.7854234	-97.80247193	1940.107637	-383.9315519
2.75						-404.964998
2.7	798.7198534	1.986819518	1449.000791	-28.75535419	2837.806718	-427.7045099
2.65						-452.1200471
2.6	1274.038338	114.4072121	2202.267793	86.99136843	4088.730441	-477.7996789
2.55	1981.787505	299.0591678	3289.333147	270.6519336	5812.828576	-503.645656
2.5						-527.5109847
2.48						-535.6846662
2.46						-542.6052924
2.44						-547.858894
2.42						-550.9601198
2.4	3026.15092	591.2525441	4844.66527	553.3543969	8159.065751	-551.3405893
2.35						-535.8204901
2.3	4554.666033	1041.85421	7051.043338	983.3954182	11301.54368	-485.7779052
2.25						-383.5749442
2.2	6774.441229	1724.773315	10152.46856	1639.987097	15418.90064	-206.4118314
2.15						74.60782946
2.1	9972.741845	2749.179082	14465.06109	2656.945076	20646.17596	497.3639691

2.05						1120.573424
2	14540.37124	4279.682904	20378.64004	4258.748299	27027.87608	2051.564691
1.9	20992.25284	6569.031729	28334.44084	6809.522345	34611.50614	5268.657287
1.8	29969.84152	10005.40007	38763.19281	10887.76338	43526.96896	10848.64397

TABLE S.9: Results of CCSD(T) calculation for Ne–RG diatomics

	Ar	Kr	Xe
R, Å	Energy, cm^{-1}		
25	-0.000365238	-0.000490207	-0.000748941
22	-0.000820376	-0.001094692	-0.001709793
20	-0.001464197	-0.002009634	-0.003011856
17	-0.003884056	-0.005450566	-0.008068751
15	-0.008370962	-0.011693338	-0.017220854
12	-0.032480879	-0.045472612	-0.066937246
10	-0.098733197	-0.138620517	-0.204960364
9	-0.188445148	-0.265164082	-0.393585811
8	-0.390180173	-0.550783215	-0.821966853
7	-0.897330728	-1.273760733	-1.917103475
6	-2.392831014	-3.405431613	-5.191070688
5.5	-4.1746992	-5.977645161	-9.15346516
5.3	-5.295991813	-7.599260148	-11.63398769
5.2	-5.98740332	-8.596131149	-13.14731815
5.1	-6.785888969	-9.743558595	-14.87605056
5	-7.709560465	-11.06518424	-16.84712759
4.9	-8.779330157	-12.58750007	-19.08883038
4.8	-10.01993092	-14.33904642	-21.6230363
4.7	-11.45470577	-16.35167922	-24.46883879
4.6	-13.11449533	-18.65394157	-27.63696074
4.5	-15.03073923	-21.2752353	-31.11434027
4.4	-17.24167121	-24.23575741	-34.85622063
4.3	-19.78058293	-27.54581678	-38.76424666
4.2	-22.67612944	-31.18661787	-42.64619462
4.1	-25.94255087	-35.09603217	-46.22155296
4	-29.55894403	-39.13958383	-48.95751966
3.9	-33.45736549	-43.05858557	-50.07728359
3.8	-37.48150192	-46.4109614	-48.37976076
3.7	-41.33477604	-48.47031694	-42.06508323
3.6	-44.49472124	-48.08891546	-28.47434569
3.5	-46.0857321	-43.49219246	-3.716287516
3.4	-44.70121115	-31.97218737	37.87267363
3.3	-38.12811396	-9.431007707	104.4972694
3.2	-22.93405292	7.790345039	207.9667597
3.1	6.178925521	30.28325629	365.1377457
3	57.3219723	59.29608774	599.8723532

2.9	142.7827381	96.34641415	945.7465158
2.8	280.9955838	143.2746488	1449.843352
2.7	499.4624004	202.3080269	2177.945485
2.6	839.088736	368.0083516	3221.349367
2.5	1360.444482	622.3237807	4705.5756
2.4	2152.703382	1007.121368	6801.747749
2.3	3346.442675	1582.875416	9741.84713
2.2	5131.841862	2436.462938	13837.76378
2.1	7784.268898	3691.931133	19502.60364
2	11699.61265	5525.431899	27273.761
1.9	17441.13482	8185.756122	37838.72839
1.8	25797.61467	12021.67478	52067.41927

II. POTENTIALS. COMPARISON TO PREVIOUS *AB INITIO* AND EXPERIMENTAL DATA

Table S.10 compares the equilibrium parameters of the present *ab initio* potentials with the selected literature results. Avoiding the complete coverage of the literature, which for some atoms is enormous, we tried to pick up the most recent and accurate *ab initio* data of the CCSD(T) level, empirical fits to experimental data and results of the Tang-Toennies (TT) model. References to earlier works can be retrieved from the citations provided. At least for half of the atoms (H, He, Li, O, Ne) literature data certify reasonably good quality of our interaction potentials. The V_Σ B-RG and F-RG potentials show large disagreement with available data. The latter case was elaborated by Hoffman and Colletto[101], who showed that the single-reference coupled-cluster approach is insufficient neglecting the coupling between the covalent and ionic $^2\Sigma$ states. Much better agreement with experimental data was achieved by using the multireference methods that accounts for strong spin-orbit coupling. The case of B-RG may deserve additional study. Little or no data exist to support our results for interactions involving Be, C and N atoms.

Overall, we believe that the present potentials are good enough to represent the trends in interaction range and energy across the first- and second-row atoms. It is not certainly true for atomic F, but we are considering this case as a hypothetical system rather than a model for real atom.

TABLE S.10. Equilibrium parameters R_e (Å) and D_e (cm^{-1}) of A-RG interaction potentials.

Atom	Potential	Source	Ar		Kr		Xe	
			R_e	D_e	R_e	D_e	R_e	D_e
H	V_Σ	present	3.60	34	3.68	42	3.81	52
		CCSD(T) Ref. 86	3.65	28	3.75	35	3.90	42
		TT Ref. 87	3.55	38	3.65	47	3.81	50
He	V_Σ	present	3.49	21	3.70	21	4.00	20
		CCSD(T) Refs. 88,89			3.71	21	3.97	20
		TT Ref. 90	3.50	21	3.69	21	3.97	20
		empirical[a]	3.48	21	3.69	21	3.98	20
Li	V_Σ	present	4.89	41	4.84	65	4.87	98
		CCSD(T) Ref. 83	4.91	41	4.82	66	4.85	99
		empirical[b]	4.89	42	4.78	68	4.80	102
Be	V_Σ	present	4.23	67	4.29	92	4.39	124
B	V_Σ	present	3.94	75	4.00	102	4.10	138
		CCSD(T) Ref. 115	4.43	45	4.50	60	4.70	68
		CCSD(T)[c]	4.38	50	4.47	65	4.59	86
	V_Π	present	3.57	126	3.60	173	3.65	243
		CCSD(T) Ref. 115	3.62	110	3.67	147	3.73	197
		CCSD(T)[c]	3.57	124	3.61	170	3.66	238
	V_0	present	4.37	52	4.42	71	4.55	92
C	V_Σ	present, Ref. 56	3.07	212	3.04	323	2.88	607
		CCSD(T) Ref. 95	3.21	150				
	V_Π	present, Ref. 56	3.93	65	4.00	81	4.15	100
	V_0	present, Ref. 56	3.73	78	3.81	101	3.94	129
N	V_Σ	present	3.62	71	3.73	85	3.92	99
O	V_Σ	present, Refs. 35,96,97	3.78	49	3.92	58	4.13	66
		CCSD(T) Refs. 98,99	3.81	46	3.94	54	4.16	58
		empirical[d]	3.85	41	4.05	45	4.24	56
	V_Π	present, Refs. 35,96,97	3.36	88	3.44	106	3.57	130
		CCSD(T) Refs. 98,99	3.36	83	3.41	100	3.68	105
		empirical[d]	3.45	84	3.57	106	3.69	140
	V_0	present, Refs. 35,96,97	3.55	65	3.65	78	3.84	91
		empirical[d]	3.60	63	3.75	75	3.90	95
F	V_Σ	present	3.07	113	3.07	154	2.45	551
		CCSD(T) Ref. 101	3.22	72	3.14	127	2.39	524
		empirical[e]	3.12	97	2.83	381	2.31	1305
	V_Π	present	3.60	50	3.76	55	3.97	59
		empirical[e]	3.61	47	3.85	46	3.93	55
	V_0	present	3.47	58	3.62	66	3.81	74
		empirical[e]	3.50	55	3.65	58	3.78	65
Ne	V_Σ	present	3.47	46	3.62	49	3.81	50
		CCSD(T) Refs. 81,89	3.49	46			3.89	51
		TT Ref. 90	3.48	46	3.65	49	3.89	49
		empirical[f]	3.49	47	3.63	50	3.86	50

[a] Fits to differential cross section and diffusion coefficients[91].
[b] Spectroscopy for Li-Ar[92], fits to differential cross sections for Li-Kr,Xe[93].
[c] Most accurate results from Ref. 94 are quoted.
[d] Fits to scattering cross sections[100].
[e] Fits to scattering cross sections[102].
[f] Fits to scattering cross sections and second virial coefficients[103].

III. TABULATED CONVEX HULLS AND FORMATION ENERGIES OF DIFFERENT VARIANTS OF IS SITE. ISOFTROPIC MODEL

TABLE S.10. Lowest energy trapping site formation energies (in cm^{-1}), obtained within the isotropic model for all atoms in Ar crystal

	Formation energy, cm^{-1}					
N deleted	0	1	2	3	4	5
H	791	151	736	1241	1685	2103
He	704	368	940	1429	1858	2274
Li	2937	806	1184	1186	990	1465
Be	2004	-214	352	786	804	1316
B	1820	-595	31	569	977	1466
C	1390	-606	28	581	1055	1466
N	1173	-407	213	759	1256	1691
O	986	-272	331	856	1315	1730
F	839	-118	480	994	1456	1865
Ne	903	45	634	1140	1600	2028

TABLE S.11. Lowest energy trapping site formation energies (in cm^{-1}), obtained within the isotropic model for all atoms in Kr crystal

	Formation energy, cm^{-1}					
N deleted	0	1	2	3	4	5
H	607	392	1227	1943	2607	3195
He	784	665	1484	2185	2848	3398
Li	2471	86	851	1316	1394	2114
Be	2736	-552	333	1084	1578	2291
B	1814	-725	205	996	1677	2269
C	1285	-518	374	1147	1819	2414
N	1146	-203	667	1416	2085	2680
O	903	-31	816	1545	2209	2781
F	812	165	1008	1730	2395	2963
Ne	1003	346	1182	1897	2526	3147

TABLE S.12. Lowest energy trapping site formation energies (in cm^{-1}), obtained within the isotropic model for all atoms in Xe crystal

	Formation energy, cm^{-1}					
N deleted	0	1	2	3	4	5
H	351	747	1914	2911	3867	4703
He	893	1065	2219	3205	4141	4923
Li	1934	-420	780	1772	2256	3270
Be	2740	-703	563	1660	2603	3457
B	1450	-659	598	1684	2636	3504
C	936	-260	965	2013	2958	3786
N	1033	158	1357	2382	3284	4129
O	721	356	1529	2520	3459	4244
F	687	579	1749	2748	3685	4467
Ne	1092	757	1925	2921	3859	4639

TABLE S.13. Formation energies (in cm^{-1}) of different variants of IS trapping site within the isotropic approximation. In Xe crystal, all atoms have IS(O_h) site as the most stable

Atom	IS(O_h)		IS(DB)		IS(SI)	
	Ar	Kr	Ar	Kr	Ar	Kr
Li	3160	2471	2937			
Be	2765	2795		2736	2004	
B	1940	1867		1814	1820	
C	1395	1285	1390			

IV. TABULATED CONVEX HULLS AND FORMATION ENERGIES OF DIFFERENT VARIANTS OF IS SITE. NR DIM MODEL

TABLE S.14. Lowest energy trapping site formation energies (in cm^{-1}), obtained within the NR DIM model for all atoms in Ar crystal

	Formation energy, cm^{-1}					
N deleted	0	1	2	3	4	5
B	1358	-674	-147	338	820	1220
C	523	-635	-19	502	978	1423
O	834	-274	327	849	1314	1728
F	656	-119	475	983	1456	1851

TABLE S.15. Lowest energy trapping site formation energies (in cm^{-1}), obtained within the NR DIM model for all atoms in Kr crystal

	Formation energy, cm^{-1}					
N deleted	0	1	2	3	4	5
B	1220	-776	64	816	1480	2106
C	78	-533	344	1023	1705	2338
O	714	-28	817	1544	2198	2828
F	501	163	990	1706	2370	2932

TABLE S.16. Lowest energy trapping site formation energies (in cm^{-1}), obtained within the NR DIM model for all atoms in Xe crystal

	Formation energy, cm^{-1}					
N deleted	0	1	2	3	4	5
B	730	-687	531	1603	2558	3409
C	-1121	-369	802	1561	2525	3301
O	474	353	1518	2516	3459	4249
F	-1428	-140	988	1929	2831	3628

TABLE S.17. Formation energies (in cm^{-1}) of different variants of IS trapping site within the NR DIM model. For O@RG IS(D_{2h}) site is unstable.

Atom	IS(O_h)			IS(D_{2h})		
	Ar	Kr	Xe	Ar	Kr	Xe
B	1485	1220	730	1358	1230	937
C	952	628	-212	514	73	-1124
O	834	714	473			
F	652	512	-178	660	500	-1429

V. STRUCTURE OF STABLE TRAPPING SITES. ISOTROPIC MODEL

TABLE S.18. Minimum O–RG distances (Å) in the IS(O_h) site optimized using the isotropic model in comparison with the equivalent distances in the ideal lattice. The number of equivalent RG atoms is given in parentheses.

RG	crystal	isotropic
	H@RG	
Ar	2.66(6)	2.93(6)
Kr	2.84(6)	3.03(6)
Xe	3.07(6)	3.19(6)
	He@RG	
Ar	2.66(6)	2.89(6)
Kr	2.84(6)	3.03(6)
Xe	3.07(6)	3.22(6)
	Li@RG	
Ar	2.66(6)	3.26(6)
Kr	2.84(6)	3.22(6)
Xe	3.07(6)	3.37(6)
	Be@RG	
Ar	2.66(6)	3.44(6)
Kr	2.84(6)	3.49(6)
Xe	3.07(6)	3.60(6)
	B@RG iso	
Ar	2.66(6)	3.31(6)
Kr	2.84(6)	3.37(6)
Xe	3.07(6)	3.47(6)
	C@RG iso	
Ar	2.66(6)	3.20(6)
Kr	2.84(6)	3.27(6)
Xe	3.07(6)	3.39(6)
	N@RG	
Ar	2.66(6)	3.13(6)
Kr	2.84(6)	3.22(6)
Xe	3.07(6)	3.37(6)
	O@RG iso	
Ar	2.66(6)	3.07(6)
Kr	2.84(6)	3.16(6)
Xe	3.07(6)	3.31(6)
	F@RG iso	
Ar	2.66(6)	3.03(6)
Kr	2.84(6)	3.13(6)
Xe	3.07(6)	3.28(6)
	Ne@RG	
Ar	2.66(6)	3.01(6)
Kr	2.84(6)	3.13(6)
Xe	3.07(6)	3.30(6)

TABLE S.19. Minimum O–RG distances (Å) in the SS site optimized using the isotropic model in comparison with the equivalent distances in the ideal lattice. The number of equivalent RG atoms is given in parentheses.

RG	crystal	isotropic
H@RG		
Ar	3.76(12)	3.72(12)
Kr	4.01(12)	3.98(12)
Xe	4.34(12)	4.28(12)
He@RG		
Ar	3.76(12)	3.72(12)
Kr	4.01(12)	3.98(12)
Xe	4.34(12)	4.31(12)
Li@RG		
Ar	3.76(12)	3.91(12)
Kr	4.01(12)	4.08(12)
Xe	4.34(12)	4.36(12)
Be@RG		
Ar	3.76(12)	3.85(12)
Kr	4.01(12)	4.04(12)
Xe	4.34(12)	4.32(12)
B@RG iso		
Ar	3.76(12)	3.77(12)
Kr	4.01(12)	3.99(12)
Xe	4.34(12)	4.29(12)
C@RG iso		
Ar	3.76(12)	3.73(12)
Kr	4.01(12)	3.97(12)
Xe	4.34(12)	4.29(12)
N@RG		
Ar	3.76(12)	3.72(12)
Kr	4.01(12)	3.96(12)
Xe	4.34(12)	4.29(12)
O@RG iso		
Ar	3.76(12)	3.71(12)
Kr	4.01(12)	3.96(12)
Xe	4.34(12)	4.29(12)
F@RG iso		
Ar	3.76(12)	3.71(12)
Kr	4.01(12)	3.97(12)
Xe	4.34(12)	4.29(12)
Ne@RG		
Ar	3.76(12)	3.71(12)
Kr	4.01(12)	3.98(12)
Xe	4.34(12)	4.30(12)

TABLE S.20. Minimum O–RG distances (Å) in the IS(DB) and IS(SI) sites optimized using the isotropic model, which are compared to the distances corresponding to equivalent positions if atom was being placed in either IS(O_h) or SS site in the ideal unperturbed lattice. The number of equivalent RG atoms is given in parentheses.

RG	crystal IS(O_h)	IS(DB)	IS(SI)	crystal SS
		Li@RG		
Ar	2.66(6)	-	3.99(2), 4.01(1), 4.05(10)	3.76(12)
		Be@RG		
Ar	2.66(6)	-	3.92(2), 3.97(10), 3.99(1)	3.76(12)
Kr	2.84(6)	3.36(1), 3.53(4), 3.84(1)	-	4.01(12)
		B@RG iso		
Ar	2.66(6)	-	3.84(2), 3.93(10), 3.97(1)	3.76(12)
Kr	2.84(6)	3.29(1), 3.38(4), 3.49(1)	-	4.01(12)
		C@RG iso		
Ar	2.66(6)	3.11(1), 3.22(4), 3.43(1)	-	3.76(12)

TABLE S.21. Minimum O–RG distances (Å) in the optimized TV site structure in comparison with the equivalent distances in the ideal lattice. The number of equivalent RG atoms is given in parentheses.

System	crystal	isotropic
Li@Ar	4.40(12)	4.42(12)
Be@Ar	4.40(12)	4.35(12)

VI. STRUCTURE OF STABLE TRAPPING SITES. NR DIM MODEL

TABLE S.22. Minimum O–RG distances (Å) in the IS(O_h) site optimized using the isotropic and NR models in comparison with the equivalent distances in the ideal lattice. The number of equivalent RG atoms is given in parentheses.

RG	crystal	isotropic	NR
		B@RG	
Ar	2.66(6)	3.31(6)	3.12(4), 3.52(2)
Kr	2.84(6)	3.37(6)	3.18(4), 3.58(2)
Xe	3.07(6)	3.47(6)	3.27(4), 3.70(2)
		C@RG	
Ar	2.66(6)	3.20(6)	2.85(2), 3.29(4)
Kr	2.84(6)	3.27(6)	2.86(2), 3.37(4)
Xe	3.07(6)	3.39(6)	2.83(2), 3.52(4)
		O@RG	
Ar	2.66(6)	3.07(6)	2.98(4), 3.20(2)
Kr	2.84(6)	3.16(6)	3.06(4), 3.29(2)
Xe	3.07(6)	3.31(6)	3.20(4), 3.45(2)
		F@RG	
Ar	2.66(6)	3.03(6)	2.81(2), 3.09(4)
Kr	2.84(6)	3.13(6)	2.65(2), 3.47(4)
Xe	3.07(6)	3.28(6)	2.33(1), 3.42(4), 3.91(1)

TABLE S.23. Minimum O–RG distances (Å) in the IS(D_{2h}) site optimized using the isotropic and NR models in comparison with the equivalent distances in the ideal lattice. The number of equivalent RG atoms is given in parentheses.

RG	crystal	NR
	B@RG	
Ar	1.88(2), 3.25(4)	3.00(2), 3.35(2), 3.62(2)[a]
Kr	2.01(2), 3.47(4)	3.02(2), 3.60(4)
Xe	2.17(2), 3.75(4)	3.06(2), 3.78(4)
	C@RG	
Ar	1.88(2), 3.25(4)	2.71(2), 3.47(4)
Kr	2.01(2), 3.47(4)	2.69(2), 3.60(4)
Xe	2.17(2), 3.75(4)	2.65(2), 3.80(4)
	F@RG	
Ar	1.88(2), 3.25(4)	2.66(2). 3.30(4)
Kr	2.01(2), 3.47(4)	2.65(2), 3.47(4)
Xe	2.17(2), 3.75(4)	2.35(2), 3.75(4)

[a] Although the structure is differently distorted from the case of C and F, it is still IS D2h

TABLE S.24. Minimum O–RG distances (Å) in the SS site optimized using the isotropic and NR models in comparison with the equivalent distances in the ideal lattice. The number of equivalent RG atoms is given in parentheses.

RG	crystal	isotropic	NR
		B@RG	
Ar	3.76(12)	3.77(12)	3.68(6), 3.85(6)
Kr	4.01(12)	3.99(12)	3.92(6), 4.05(6)
Xe	4.34(12)	4.29(12)	4.24(6), 4.33(6)
		C@RG	
Ar	3.76(12)	3.73(12)	3.56(2), 3.76(10)
Kr	4.01(12)	3.97(12)	3.94(8), 4.01(4)
Xe	4.34(12)	4.29(12)	3.05(1), 3.98(4), 4.38(2), 4.88(4), 5.30(1)
		O@RG	
Ar	3.76(12)	3.71(12)	3.68(6), 3.74(6)
Kr	4.01(12)	3.96(12)	3.94(4), 3.98(8)
Xe	4.34(12)	4.29(12)	4.28(4), 4.30(8)
		F@RG	
Ar	3.76(12)	3.71(12)	3.70(8), 3.73(4)
Kr	4.01(12)	3.97(12)	3.96(8), 3.98(4)
Xe	4.34(12)	4.29(12)	4.29(8), 4.30(4)

VII. CALCULATED VIBRATIONAL FREQUENCES OF CENTRAL ATOM WITHIN ALL STABLE TRAPPING SITES

TABLE S.25. Central atom vibrational frequences for IS(O_h) sites within Einstein aproximation for isotropic and NR DIM models

RG	isotropic	NR
	H@RG	
Ar	332, 332, 332	
Kr	337, 337, 337	
Xe	316, 316, 316	
	He@RG	
Ar	182, 182, 182	
Kr	187, 187, 187	
Xe	187, 187, 187	
	Li@RG	
Ar	76, 76, 76	
Kr	70, 70, 70	
Xe	83, 83, 83	
	Be@RG	
Ar	130, 130, 130	
Kr	140, 140, 140	
Xe	148, 148, 148	
	B@RG	
Ar	127, 127, 127	126, 126, 141
Kr	134, 134, 134	131, 131, 154
Xe	140, 140, 140	132, 132, 165
	C@RG	
Ar	125, 125, 125	119, 136, 136
Kr	132, 132, 132	122, 146, 146
Xe	135, 135, 135	125, 158, 158
	N@RG	
Ar	117, 117, 117	
Kr	124, 124, 124	
Xe	126, 126, 126	
	O@RG	
Ar	109, 109, 109	107, 107, 116
Kr	114, 114, 114	109, 109, 123
Xe	114, 114, 114	104, 104, 129
	F@RG	
Ar	99, 99, 99	91, 104, 104
Kr	103, 103, 103	84, 109, 109
Xe	101, 101, 101	45, 127, 127
	Ne@RG	
Ar	96, 96, 96	
Kr	99, 99, 99	
Xe	101, 101, 101	

TABLE S.26. Central atom vibrational frequences for IS(D_{2h}) sites within Einstein aproximation for NR DIM model

RG	Frequences, cm^{-1}
B@RG	
Ar	73, 120, 169
Kr	57, 119, 186
Xe	46, 111, 120
C@RG	
Ar	82, 120, 168
Kr	88, 126, 185
Xe	106, 136, 218
F@RG iso	
Ar	45, 75, 137
Kr	51, 77, 139
Xe	117, 126, 225

TABLE S.27. Central atom vibrational frequences for IS(DB) sites within Einstein aproximation for isotropic model

RG	Frequences, cm^{-1}
Be@RG	
Kr	129, 129, 151
B@RG iso	
Kr	130, 130, 138
C@RG iso	
Ar	116, 116, 131

TABLE S.28. Central atom vibrational frequences for IS(SI) sites within Einstein aproximation for isotropic model

RG	Frequences, cm^{-1}
Li@RG	
Ar	88, 89, 89
Be@RG	
Ar	93, 93, 96
B@RG iso	
Ar	64, 67, 73

VIII. PREEXPONENTS ν USED IN STST CALCULATIONS

TABLE S.29. Approximate vibrational frequences of the mode directed along the IS(O_h)–IS*(D_{2h})–IS(O_h) migration path and the preexponents ν used in STST calculations within the isotropic model.

	$\omega(\mathrm{cm}^{-1})$	$\nu(\mathrm{s}^{-1})$
H@RG		
Ar	333	9.97×10^{12}
Kr	337	1.01×10^{13}
Xe	316	9.48×10^{12}
D@RG		
Ar	236	7.08×10^{12}
Kr	239	7.17×10^{12}
Xe	234	7.02×10^{12}
He@RG		
Ar	182	5.46×10^{12}
Kr	186	5.59×10^{12}
Xe	187	5.62×10^{12}
Li@RG		
Kr	70	2.09×10^{12}
Xe	83	2.48×10^{12}
Be@RG		
Xe	148	4.44×10^{12}
B@RG		
Kr	133	3.99×10^{12}
Xe	140	4.21×10^{12}
C@RG		
Ar	124	3.72×10^{12}
Kr	132	3.95×10^{12}
Xe	135	4.04×10^{12}
N@RG		
Ar	117	3.51×10^{12}
Kr	124	3.72×10^{12}
Xe	126	3.79×10^{12}
O@RG		
Ar	109	3.26×10^{12}
Kr	114	3.42×10^{12}
Xe	113	3.39×10^{12}
F@RG		
Ar	99	2.98×10^{12}
Kr	103	3.08×10^{12}
Xe	102	3.05×10^{12}
Ne@RG		
Ar	96	2.88×10^{12}
Kr	99	2.98×10^{12}
Xe	101	3.03×10^{12}

TABLE S.30. Approximate vibrational frequences of the mode directed along the migration path and the preexponents ν used in STST calculations within the NR DIM model.

	Path type	$\omega(\mathrm{cm}^{-1})$	$\nu(\mathrm{s}^{-1})$
	B NR		
Ar	IS(D_{2h})-IS(O_h)-IS(D_{2h})	74	2.21×10^{12}
Kr	IS(O_h)-IS(D_{2h})-IS(O_h)	131	3.93×10^{12}
Xe	IS(O_h)-IS(D_{2h})-IS(O_h)	149	4.47×10^{12}
	C NR		
Ar	IS(D_{2h})-IS(O_h)-IS(D_{2h})	82	2.45×10^{12}
Kr	IS(D_{2h})-IS(O_h)-IS(D_{2h})	88	2.65×10^{12}
Xe	IS(D_{2h})-IS*-IS(D_{2h})	136	4.09×10^{12}
	O NR		
Ar	IS(O_h)-IS*(D_{2h})-IS(O_h)	112	3.35×10^{12}
Kr	IS(O_h)-IS*(D_{2h})-IS(O_h)	117	3.50×10^{12}
Xe	IS(O_h)-IS*(D_{2h})-IS(O_h)	116	3.49×10^{12}