Supporting Information: Accurate atomic correlation and total energies for correlation consistent effective core potentials

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1 Data in D_{2h} point group

Tables S1, S2, S3, S4, S5, S6, and S7 provide energies in D_{2h} point group for various elements and pseudopotentials. Tables S8, S9, S10, S11, S12, and S13 provide the corresponding kinetic energies in D_{2h} point group.

Table S1: Atomic correlation and total energies [Ha] for the 1st-row elements with ccECPs[He] for indicated basis sets and methods in D_{2h} point group. Post-HF method values correspond to correlation energies. CBS denotes basis set extrapolated values. Values with (*) were not feasible to calculate and represent estimates from the calculated data. aug-cc-pVnZ basis set (cc-pVnZ for Ne).

Atom	Method	DZ	TZ	QZ	5Z	6Z	CBS
H	ROHF	-0.49999965	-0.49999965	-0.49999965	-0.49999965		-0.49999965(1)
	CISD	-0.03390801	-0.03946245	-0.04103940	-0.04156934	-0.04177354	-0.042065(23)
He	RHF	-2.86167947	-2.86167947	-2.86167948	-2.86167948	-2.86167948	-2.86167948(1)
	Total						-2.903745(23)
Li	ROHF	-0.19685279	-0.19685279	-0.19685279	-0.19685279		-0.19685279(1)
	CISD	-0.04699395	-0.04781761	-0.04806189	-0.04818173	-0.04824394	-0.04834636(12)
Be	RHF	-0.96189258	-0.96189258	-0.96189258	-0.96189259	-0.96189258	-0.96189260(2)
	Total						-1.01023896(12)
	CISD	-0.06484682	-0.07153471	-0.07300263	-0.07333752	-0.07355788	-0.07369(12)
	RCCSD(T)	-0.06593395	-0.07322628	-0.07482123	-0.07518494	-0.07542931	-0.07558(13)
	UCCSD(T)	-0.06594278	-0.07327882	-0.07487428	-0.07523735	-0.07548152	-0.07563(13)
B	FCI	-0.06633674	-0.07374227	-0.07529726	-0.07564267	-0.07587512	-0.07601(13)
	ROHF	-2.53929199	-2.53929951	-2.53930397	-2.53930456	-2.53930597	-2.539306(1)
	Total						-2.61531(13)
	CISD	-0.07855565	-0.09409202	-0.09742648	-0.09824707	-0.09879999	-0.09919(28)
	RCCSD(T)	-0.08030708	-0.09708463	-0.10069041	-0.10157747	-0.10218081	-0.10261(31)
	UCCSD(T)	-0.08034503	-0.09722437	-0.10083382	-0.10172039	-0.10232381	-0.10275(31)
C	CCSDT(Q)	-0.08074613	-0.09777804	-0.10134593	-0.10220841	-0.10279602	-0.10320(31)
	FCI	-0.08075703	-0.09778825	-0.10135573	-0.10221784	-0.10280522	-0.10321(31)
	ROHF	-5.31430315	-5.31431227	-5.31431802	-5.31431738	-5.31431979	-5.314320(2)
	Total						-5.41753(31)
	CISD	-0.09359382	-0.11782215	-0.12363123	-0.12539949	-0.12617272	-0.127077(65)
	RCCSD(T)	-0.09564583	-0.12165286	-0.12789000	-0.12977963	-0.13061050	-0.131573(76)
	UCCSD(T)	-0.09570506	-0.12185906	-0.12811222	-0.12999924	-0.13083009	-0.131786(79)
N	CCSDT(Q)	-0.09598629	-0.12230085	-0.12852942	-0.13038605	-0.13120254	-0.132125(84)
	FCI	-0.09599171	-0.12230706	-0.12853580	-0.13039205	-0.131208(*)	-0.132131(85)
	ROHF	-9.63386641	-9.63386651	-9.63386735	-9.63386820	-9.63386789	-9.6338682(9)
	Total						-9.765999(85)
	CISD	-0.1246492	-0.1661684	-0.1782075	-0.1821435	-0.1839430	-0.18621(14)
	RCCSD(T)	-0.1285665	-0.1728490	-0.1856582	-0.1897979	-0.1917074	-0.19407(18)
	UCCSD(T)	-0.1286637	-0.1730425	-0.1858716	-0.1900124	-0.1919217	-0.19428(18)
O	CCSDT(Q)	-0.1289799	-0.1734730	-0.1862864	-0.1903987	-0.1922914	-0.19462(18)
	FCI	-0.1289761	-0.1734721	-0.1862864	-0.1903(*)	-0.1922(*)	-0.19462(18)
	ROHF	-15.6887438	-15.6896444	-15.6897753	-15.6897740	-15.6897920	-15.68979(2)
	Total						-15.88441(18)
	CISD	-0.16290810	-0.21762589	-0.23569494	-0.24149765	-0.24449739	-0.24799(57)
	RCCSD(T)	-0.16862537	-0.22701406	-0.24616290	-0.25226239	-0.25543329	-0.25908(63)
	UCCSD(T)	-0.16869113	-0.22713392	-0.24629766	-0.25239795	-0.25556974	-0.25922(63)
F	CCSDT(Q)	-0.16895239	-0.22745581	-0.24660080	-0.25267684	-0.2559(*)	-0.25948(65)
	FCI	-0.16894606	-0.22744583				
	ROHF	-23.93700527	-23.93782831	-23.93791497	-23.93791376	-23.93792456	-23.937925(9)
	Total						-24.19741(65)
	CISD	-0.18025458	-0.24989860	-0.29174759	-0.30201083	-0.30627967	-0.30949(91)
	RCCSD(T)	-0.18462256	-0.25961485	-0.30453033	-0.31557498	-0.32014022	-0.32361(94)
	UCCSD(T)	-0.18462256	-0.25961472	-0.30453031	-0.31557497	-0.32014021	-0.32361(94)
Ne	CCSDT(Q)	-0.18480612	-0.25973913	-0.30463859	-0.31566443	-0.3202(*)	-0.32368(96)
	RHF	-34.70881857	-34.70881857	-34.70881857	-34.70881857	-34.70881857	-34.70881857(3)
	Total						-35.03250(96)

Table S2: Atomic correlation and total energies [Ha] for selected elements with BFD ECPs in D_{2h} point group. Notations as in table S1. aug-cc-pVnZ basis set.

Atom	Method	DZ	TZ	QZ	5Z	6Z	CBS
	CISD	-0.08218682	-0.09634560	-0.09937206	-0.10014903	-0.10072325	-0.10116(30)
	RCCSD(T)	-0.08412432	-0.09947264	-0.10276136	-0.10359700	-0.10422630	-0.10469(34)
	UCCSD(T)	-0.08416583	-0.09961460	-0.10290812	-0.10374218	-0.10437165	-0.10484(34)
C	CCSDT(Q)	-0.08460615	-0.10018697	-0.10343924	-0.10424590	-0.10485861	-0.10530(34)
	FCI	-0.08461818	-0.10019762	-0.10344958	-0.10425580	-0.10486826	-0.10531(34)
	ROHF	-5.32901824	-5.32902791	-5.32903304	-5.32903242	-5.32903425	-5.329034(2)
	Total						-5.43434(34)
	CISD	-0.09671731	-0.12005299	-0.12559499	-0.12724555	-0.12802543	-0.12888(13)
	RCCSD(T)	-0.09894790	-0.12402643	-0.12998438	-0.13174854	-0.13258862	-0.13350(15)
	UCCSD(T)	-0.09900824	-0.12423526	-0.13020784	-0.13196952	-0.13280967	-0.13371(15)
N	CCSDT(Q)	-0.09930931	-0.12469007	-0.13063388	-0.13236535	-0.13319069	-0.13406(15)
	FCI	-0.09931577	-0.12469623	-0.13064048	-0.13237147	-0.133197(*)	-0.13407(15)
	ROHF	-9.66837630	-9.66837630	-9.66837630	-9.66837632	-9.66837636	-9.6683764(2)
	Total						-9.80244(15)
	CISD	-0.1316691	-0.1708663	-0.1821616	-0.1859531	-0.1877270	-0.19001(14)
	RCCSD(T)	-0.1361045	-0.1779572	-0.1899846	-0.1939762	-0.1958616	-0.19826(18)
	UCCSD(T)	-0.1362079	-0.1781587	-0.1902053	-0.1941977	-0.1960834	-0.19849(19)
O	CCSDT(Q)	-0.1365493	-0.1786065	-0.1906330	-0.1945964	-0.1964645	-0.19887(20)
	FCI	-0.1365476	-0.1786048	-0.1906327	-0.1945(*)	-0.1964(*)	-0.19887(20)
	ROHF	-15.7074522	-15.7083474	-15.7084813	-15.7084799	-15.7084963	-15.70850(2)
	Total						-15.90737(20)
	CISD	-0.06971290	-0.08096003	-0.08330143	-0.08393851	-0.08431909	-0.08465(15)
	RCCSD(T)	-0.07168674	-0.08462009	-0.08737082	-0.08811695	-0.08855472	-0.08894(16)
	UCCSD(T)	-0.07172215	-0.08485851	-0.08761415	-0.08835626	-0.08879496	-0.08917(17)
Si	CCSDT(Q)	-0.07227756	-0.08575195	-0.08844280	-0.08913078	-0.08954322	-0.08987(17)
	FCI	-0.07229743	-0.08577362	-0.08846507	-0.08915166	-0.08956355	-0.08988(17)
	ROHF	-3.67867214	-3.67867292	-3.67867531	-3.67867557	-3.67867577	-3.6786758(2)
	Total						-3.76856(17)

Table S3: Atomic correlation and total energies [Ha] for the 2nd-row elements with ccECPs[Ne] in D_{2h} point group. Notations as in table S1. aug-cc-pVnZ basis set (cc-pVnZ for Ar).

Atom	Method	DZ	TZ	QZ	5Z	6Z	CBS
Na	ROHF	-0.18583098	-0.18615968	-0.18620499	-0.18620544		-0.1862059(2)
	CISD	-0.03375431	-0.03488593	-0.03495923	-0.03498970	-0.03503476	-0.035077(30)
Mg	RHF	-0.78825768	-0.78835857	-0.78839186	-0.78839376	-0.78839489	-0.788396(3)
	Total						-0.823473(30)
	CISD	-0.05263400	-0.05654840	-0.05751761	-0.05782447	-0.05796196	-0.058130(11)
	RCCSD(T)	-0.05372003	-0.05815196	-0.05924415	-0.05959197	-0.05974726	-0.059939(11)
	UCCSD(T)	-0.05373423	-0.05822181	-0.05931393	-0.05966124	-0.05981620	-0.060007(11)
Al	FCI	-0.05418690	-0.05874704	-0.05978600	-0.06011384	-0.06025660	-0.0604328(79)
	ROHF	-1.87708853	-1.87708645	-1.87709009	-1.87709039	-1.87709061	-1.8770907(3)
	Total						-1.9375235(79)
	CISD	-0.07148347	-0.08068087	-0.08287535	-0.08362689	-0.08390427	-0.084320(48)
	RCCSD(T)	-0.07354504	-0.08431777	-0.08689537	-0.08776849	-0.08809207	-0.088569(52)
	UCCSD(T)	-0.07358321	-0.08455595	-0.08713604	-0.08801058	-0.08833074	-0.088807(56)
Si	CCSDT(Q)	-0.07415484	-0.08544303	-0.08794586	-0.08877492	-0.08906923	-0.089501(57)
	FCI	-0.07417456	-0.08546440	-0.08796749	-0.08879555	-0.08908922	-0.089520(57)
	ROHF	-3.67255079	-3.67254920	-3.67255262	-3.67255314	-3.67255323	-3.6725533(2)
	Total						-3.762073(57)
	CISD	-0.0872674	-0.1041457	-0.1081973	-0.1095219	-0.1100142	-0.110706(64)
	RCCSD(T)	-0.0899578	-0.1098976	-0.1147390	-0.1162992	-0.1168722	-0.117667(76)
	UCCSD(T)	-0.0900033	-0.1102977	-0.1151428	-0.1167031	-0.1172737	-0.118066(78)
P	CCSDT(Q)	-0.0905108	-0.1113014	-0.1160981	-0.1175918	-0.1181241	-0.118837(74)
	FCI	-0.0905450	-0.1113280	-0.1161277	-0.1176(*)	-0.1181(*)	-0.118867(74)
	ROHF	-6.3409664	-6.3409664	-6.3409664	-6.3409664	-6.3409664	-6.3409664(1)
	Total						-6.459833(74)
	CISD	-0.1150761	-0.1477062	-0.1571694	-0.1601329	-0.1612589	-0.162730(83)
	RCCSD(T)	-0.1205488	-0.1583130	-0.1692069	-0.1726164	-0.1738859	-0.17556(12)
	UCCSD(T)	-0.1206256	-0.1586182	-0.1695648	-0.1729798	-0.1742491	-0.17592(12)
S	CCSDT(Q)	-0.1212334	-0.1596349	-0.1706112	-0.1739650	-0.1751899	-0.17676(12)
	FCI	-0.1212619	-0.1596680	-0.1706499	-0.1740(*)	-0.1752(*)	-0.17680(12)
	ROHF	-9.9189935	-9.9205928	-9.9206059	-9.9206283	-9.9206406	-9.92065(6)
	Total						-10.09745(13)
	CISD	-0.14305710	-0.19039965	-0.20634077	-0.21129242	-0.21319510	-0.21564(11)
	RCCSD(T)	-0.15050816	-0.20538895	-0.22362070	-0.22929092	-0.23142360	-0.23420(17)
	UCCSD(T)	-0.15057103	-0.20557900	-0.22386628	-0.22954346	-0.23167677	-0.23444(17)
Cl	CCSDT(Q)	-0.15113925	-0.20651142	-0.22486325	-0.23049667	-0.23263(*)	-0.23535(17)
	FCI	-0.15115932	-0.20654307				
	ROHF	-14.68992169	-14.69129790	-14.69132557	-14.69133957	-14.69134674	-14.69135(3)
	Total						-14.92670(18)
	CISD	-0.14172846	-0.22523355	-0.25200143	-0.26029839	-0.26354799	-0.26766(11)
	RCCSD(T)	-0.14635485	-0.24208710	-0.27329000	-0.28294884	-0.28664854	-0.29138(21)
	UCCSD(T)	-0.14635487	-0.24208709	-0.27329003	-0.28294886	-0.28664854	-0.29138(21)
Ar	CCSDT(Q)	-0.14660047	-0.24266875	-0.27404277	-0.28371164	-0.28736669	-0.29204(24)
	FCI	-0.14661423	-0.24268224				
	RHF	-20.77966277	-20.77966277	-20.77966277	-20.77966277	-20.77966277	-20.77966277(1)
	Total						-21.07170(24)

Table S4: Atomic correlation and total energies [Ha] for the 2nd-row elements with ccECPs[He] in D_{2h} point group. Notations as in table S1. cc-pCVnZ basis set.

Atom	Method	DZ	TZ	QZ	5Z	6Z	CBS
Na	CISD	-0.18031248	-0.27172919	-0.29544389	-0.30406634	-0.30788932	-0.313410(61)
	RCCSD(T)	-0.18344571	-0.28002589	-0.30494689	-0.31397705	-0.31797296	-0.323729(64)
	UCCSD(T)	-0.18344870	-0.28003157	-0.30495305	-0.31398332	-0.31797928	-0.323736(64)
	CCSDT(Q)	-0.18353692	-0.28010235	-0.3050(*)	-0.3141(*)	-0.3181(*)	-0.323818(64)
	ROHF	-47.35715946	-47.35715947	-47.35715947	-47.35715948	-47.35715948	-47.3571595(1)
	Total						-47.680977(64)
Mg	CISD	-0.19418640	-0.29280864	-0.32236519	-0.33189329	-0.33599570	-0.34124(12)
	RCCSD(T)	-0.20421196	-0.30991836	-0.34168720	-0.35180972	-0.35613221	-0.36159(13)
	UCCSD(T)	-0.20421197	-0.30991843	-0.34168729	-0.35180982	-0.35613232	-0.36159(13)
	CCSDT(Q)	-0.20425786	-0.31002264	-0.3418(*)	-0.3519(*)	-0.3563(*)	-0.36171(13)
	RHF	-62.92742515	-62.92742515	-62.92742515	-62.92742519	-62.92742527	-62.9274253(1)
	Total						-63.28914(13)
Al	CISD	-0.22003852	-0.31517598	-0.34527439	-0.35635744	-0.36102686	-0.36806(35)
	RCCSD(T)	-0.23228632	-0.33518844	-0.36750815	-0.37931814	-0.38427147	-0.39169(38)
	UCCSD(T)	-0.23229708	-0.33526445	-0.36759523	-0.37940692	-0.38436088	-0.39178(37)
	CCSDT(Q)	-0.23271205	-0.33579218	-0.3681(*)	-0.3800(*)	-0.3850(*)	-0.39240(38)
	ROHF	-80.99328467	-80.99334970	-80.99337935	-80.99338556	-80.99338866	-80.993389(1)
	Total						-81.38578(38)
Si	CISD	-0.2380255	-0.3416443	-0.3736974	-0.3850944	-0.3901563	-0.3972932(66)
	RCCSD(T)	-0.2506875	-0.3640548	-0.3986946	-0.4108863	-0.4162704	-0.4238033(46)
	UCCSD(T)	-0.2507063	-0.3642777	-0.3989388	-0.4111313	-0.4165151	-0.4240436(35)
	CCSDT(Q)	-0.2511863	-0.3650993	-0.3998(*)	-0.4121(*)	-0.4174(*)	-0.4250000(35)
	ROHF	-101.6261452	-101.6262120	-101.6262446	-101.6262531	-101.6262562	-101.6262569(5)
	Total						-102.0512569(35)
P	CISD	-0.2543832	-0.3690643	-0.4034612	-0.4157952	-0.4213758	-0.429233(66)
	RCCSD(T)	-0.2660361	-0.3925322	-0.4299939	-0.4432510	-0.4492035	-0.457505(72)
	UCCSD(T)	-0.2660517	-0.3928744	-0.4303578	-0.4436120	-0.4495627	-0.457855(74)
	CCSDT(Q)	-0.2664275	-0.3937591	-0.4313(*)	-0.4446(*)	-0.4506(*)	-0.458886(74)
	ROHF	-125.2587059	-125.2587059	-125.2587059	-125.2587065	-125.2587061	-125.2587067(5)
	Total						-125.717593(74)
S	CISD	-0.2793964	-0.4127255	-0.4528366	-0.4672435	-0.4736476	-0.482768(41)
	RCCSD(T)	-0.2930399	-0.4421691	-0.4865684	-0.5022234	-0.5090885	-0.518749(61)
	UCCSD(T)	-0.2930866	-0.4424431	-0.4868980	-0.5025637	-0.5094302	-0.519090(62)
	CCSDT(Q)	-0.2934939	-0.4433127	-0.4878(*)	-0.5036(*)	-0.5104(*)	-0.520110(62)
	ROHF	-151.9174562	-151.9188863	-151.9190867	-151.9191670	-151.9191789	-151.91920(1)
	Total						-152.439305(63)
Cl	CISD	-0.3055167	-0.4571395	-0.5040043	-0.5206145	-0.5282382	-0.53876(25)
	RCCSD(T)	-0.3202308	-0.4909785	-0.5433977	-0.5616090	-0.5698336	-0.58104(23)
	UCCSD(T)	-0.3202703	-0.4911532	-0.5436256	-0.5618489	-0.5700754	-0.58129(23)
	CCSDT(Q)	-0.3206352	-0.4919171	-0.5445(*)	-0.5627(*)	-0.5710(*)	-0.58219(23)
	ROHF	-181.6134018	-181.6146398	-181.6148291	-181.6148963	-181.6149016	-181.61491(1)
	Total						-182.19710(23)
Ar	CISD	-0.3291259	-0.4983511	-0.5527181	-0.5720171	-0.5808150	-0.59302(22)
	RCCSD(T)	-0.3438517	-0.5346209	-0.5956646	-0.6169443	-0.6264745	-0.63957(18)
	UCCSD(T)	-0.3438517	-0.5346209	-0.5956646	-0.6169443	-0.6264745	-0.63957(18)
	CCSDT(Q)	-0.3441534	-0.5351650	-0.5963(*)	-0.6176(*)	-0.6271(*)	-0.64022(18)
	RHF	-214.8921598	-214.8921598	-214.8921599	-214.8921604	-214.8921611	-214.8921612(8)
	Total						-215.53238(18)

Table S5: Atomic correlation and total energies [Ha] for the 3rd-row main group elements with ccECPs in D_{2h} point group. Notations as in table S1. aug-cc-pVnZ basis set (cc-pCVnZ for K, Ca).

Atom	Method	DZ	TZ	QZ	5Z	6Z	CBS
K	CISD	-0.17702362	-0.25025818	-0.27680275	-0.28486555	-0.28829755	-0.29235(21)
	RCCSD(T)	-0.18450036	-0.26859548	-0.29941325	-0.30862333	-0.31247228	-0.31694(21)
	UCCSD(T)	-0.18450996	-0.26860642	-0.29942606	-0.30863645	-0.31248545	-0.31695(21)
	CCSDT(Q)	-0.18489132	-0.26921595	-0.30016619	-0.30939(*)	-0.31325(*)	-0.31772(22)
	ROHF	-27.93462232	-27.93462232	-27.93462245	-27.93462245	-27.93462530	-27.934626(4)
	Total						-28.25235(22)
Ca	CISD	-0.22929612	-0.29416623	-0.32310943	-0.33133840	-0.33484191	-0.33854(38)
	RCCSD(T)	-0.25051655	-0.32692010	-0.36059895	-0.37009280	-0.37412840	-0.37833(46)
	UCCSD(T)	-0.25051659	-0.32692014	-0.36059897	-0.37009283	-0.37412851	-0.37833(46)
	CCSDT(Q)	-0.25129831	-0.32773983	-0.36145323	-0.37096(*)	-0.37501(*)	-0.37924(46)
	RHF	-36.34973416	-36.34973414	-36.34973418	-36.34973433	-36.34973523	-36.349736(2)
	Total						-36.72897(46)
Ga	CISD	-0.0471675	-0.0520006	-0.0532955	-0.0536905	-0.0538359	-0.054021(13)
	RCCSD(T)	-0.0479409	-0.0531965	-0.0545981	-0.0550295	-0.0551881	-0.055393(15)
	UCCSD(T)	-0.0479508	-0.0532523	-0.0546542	-0.0550851	-0.0552434	-0.055448(15)
	FCI	-0.0482426	-0.0535917	-0.0549576	-0.0553676	-0.0555165	-0.055702(13)
	ROHF	-1.9842101	-1.9842115	-1.9842118	-1.9842123	-1.9842123	-1.9842125(7)
	Total						-2.039915(13)
Ge	CISD	-0.0618893	-0.0715539	-0.0744101	-0.0751125	-0.0754253	-0.075660(82)
	RCCSD(T)	-0.0633774	-0.0743062	-0.0775083	-0.0782960	-0.0786438	-0.078905(89)
	UCCSD(T)	-0.0634057	-0.0744932	-0.0776966	-0.0784819	-0.0788279	-0.079086(89)
	CCSDT(Q)	-0.0637885	-0.0751051	-0.0782488	-0.0789902	-0.0793152	-0.079530(93)
	FCI	-0.0638013	-0.0751173	-0.0782614	-0.0790018	-0.0793264	-0.079540(94)
	ROHF	-3.6649011	-3.6649018	-3.6649020	-3.6649026	-3.6649029	-3.664903(1)
	Total						-3.744443(94)
As	CISD	-0.07039641	-0.08714420	-0.09165502	-0.09303262	-0.09360150	-0.094288(16)
	RCCSD(T)	-0.07212776	-0.09120004	-0.09632986	-0.09787671	-0.09850951	-0.099262(18)
	UCCSD(T)	-0.07215698	-0.09150397	-0.09663415	-0.09817850	-0.09880856	-0.099556(17)
	CCSDT(Q)	-0.07246222	-0.09216830	-0.09725624	-0.09874078	-0.09933940	-0.100017(24)
	FCI	-0.07248341	-0.09218100	-0.09727123	-0.09875(*)	-0.09935(*)	-0.100032(24)
	ROHF	-6.06587734	-6.06587663	-6.06587765	-6.06587778	-6.06587820	-6.0658782(4)
	Total						-6.165911(24)
Se	CISD	-0.0930417	-0.1238735	-0.1342895	-0.1372959	-0.1385311	-0.139892(82)
	RCCSD(T)	-0.0970224	-0.1316780	-0.1433240	-0.1466501	-0.1480022	-0.149470(88)
	UCCSD(T)	-0.0970916	-0.1319178	-0.1436107	-0.1469376	-0.1482886	-0.149746(91)
	CCSDT(Q)	-0.0975463	-0.1326448	-0.1443623	-0.1476235	-0.1489306	-0.150289(96)
	FCI	-0.0975657	-0.1326644	-0.1443871	-0.1476(*)	-0.1489(*)	-0.150314(96)
	ROHF	-9.1485604	-9.1499852	-9.1500304	-9.1500502	-9.1500535	-9.150058(4)
	Total						-9.300372(96)
Br	CISD	-0.1106854	-0.1539119	-0.1730843	-0.1781924	-0.1802462	-0.18219(23)
	RCCSD(T)	-0.1159228	-0.1645191	-0.1859497	-0.1916067	-0.1938530	-0.19594(25)
	UCCSD(T)	-0.1159752	-0.1646545	-0.1861409	-0.1918017	-0.1940475	-0.19612(25)
	CCSDT(Q)	-0.1164057	-0.1653027	-0.1868675	-0.1924770	-0.1947(*)	-0.19674(30)
	FCI	-0.1164173	-0.1653206				
	ROHF	-13.1201540	-13.1215071	-13.1215404	-13.1215496	-13.1215514	-13.1215524(4)
	Total						-13.31829(30)
Kr	CISD	-0.13816713	-0.18591690	-0.21246190	-0.21982064	-0.22280036	-0.22586(26)
	RCCSD(T)	-0.14505536	-0.19969369	-0.22916475	-0.23733449	-0.24060491	-0.24398(25)
	UCCSD(T)	-0.14505533	-0.19969370	-0.22916475	-0.23733449	-0.24060491	-0.24398(25)
	CCSDT(Q)	-0.14545281	-0.20023839	-0.22975824	-0.23790612	-0.24118(*)	-0.24453(27)
	FCI	-0.14546095					
	RHF	-18.22805984	-18.22806066	-18.22806022	-18.22806208	-18.22806315	-18.228065(5)
	Total						-18.47259(27)

Table S6: Atomic correlation and total energies [Ha] for Sc-Mn elements with ccECPs[Ne] in D_{2h} point group. Notations as in table S1. cc-pCVnZ basis set.

Atom	Method	DZ	TZ	QZ	5Z	CBS
Sc(^{2}D)	CISD	-0.32796256	-0.36173730	-0.37396087	-0.38010997	-0.38679(76)
	RCCSD(T)	-0.36604310	-0.40497119	-0.41878760	-0.42563016	-0.43308(80)
	UCCSD(T)	-0.36618982	-0.40514523	-0.41896722	-0.42581186	-0.43327(80)
	CCSDT(Q)	-0.36765472	-0.40664250	-0.42051(*)	-0.42738(*)	-0.43488(80)
	ROHF	-46.12178822	-46.12210462	-46.12212554	-46.12213770	-46.122138(7)
	Total					-46.55702(80)
Ti(^{3}F)	CISD	-0.35705400	-0.39826616	-0.41414637	-0.42185097	-0.43071(66)
	RCCSD(T)	-0.39748548	-0.44451483	-0.46238810	-0.47102902	-0.48093(75)
	UCCSD(T)	-0.39771070	-0.44479054	-0.46267417	-0.47132242	-0.48123(75)
	CCSDT(Q)	-0.39919402	-0.44627755	-0.46422(*)	-0.47289(*)	-0.48285(75)
	ROHF	-57.60900801	-57.60962174	-57.60970089	-57.60974274	-57.60974(2)
	Total					-58.09260(75)
V(^{4}F)	CISD	-0.39906122	-0.44502617	-0.46612164	-0.47512813	-0.48744(41)
	RCCSD(T)	-0.44481779	-0.49730050	-0.52152631	-0.53178845	-0.54594(55)
	UCCSD(T)	-0.44524393	-0.49778253	-0.52202801	-0.53229413	-0.54646(55)
	CCSDT(Q)	-0.45243936	-0.50511842	-0.52972(*)	-0.54013(*)	-0.55457(58)
	ROHF	-70.88650990	-70.88687052	-70.88703541	-70.88707243	-70.88712(3)
	Total					-71.44169(58)
Cr(^{7}S)	CISD	-0.42723842	-0.48776726	-0.51425496	-0.52577647	-0.54103(24)
	RCCSD(T)	-0.46229170	-0.53117291	-0.56131191	-0.57436463	-0.59170(32)
	UCCSD(T)	-0.46257604	-0.53151639	-0.56168036	-0.57474085	-0.59209(33)
	CCSDT(Q)	-0.46308970	-0.53189219	-0.56207(*)	-0.57514(*)	-0.59253(33)
	ROHF	-86.04808378	-86.04855303	-86.04855377	-86.04855525	-86.04856(1)
	Total					-86.64109(33)
Mn(^{6}S)	CISD	-0.4573916	-0.5221195	-0.5522082	-0.5647893	-0.58237(83)
	RCCSD(T)	-0.5044855	-0.5779711	-0.6121330	-0.6263267	-0.6463(10)
	UCCSD(T)	-0.5049472	-0.5784922	-0.6126726	-0.6268722	-0.6468(10)
	CCSDT(Q)	-0.5056657	-0.5790926	-0.61330(*)	-0.62752(*)	-0.6475(10)
	ROHF	-103.2441380	-103.2443328	-103.2443341	-103.2443426	-103.244343(6)
	Total					-103.8919(10)

Table S7: Atomic correlation and total energies [Ha] for Fe-Zn elements with ccECPs[Ne] in D_{2h} point group. Notations as in table S1. cc-pCVnZ basis set.

Atom	Method	DZ	TZ	QZ	5Z	CBS
Fe(^{5}D)	CISD	-0.5107712	-0.5884189	-0.6255361	-0.6415891	-0.66360(68)
	RCCSD(T)	-0.5650689	-0.6532492	-0.6957991	-0.7140405	-0.73932(94)
	UCCSD(T)	-0.5656015	-0.6538446	-0.6964242	-0.7146814	-0.73998(94)
	CCSDT(Q)	-0.5663308	-0.6543966	-0.69701(*)	-0.71528(*)	-0.74062(95)
	ROHF	-122.6459835	-122.6471770	-122.6472877	-122.6473522	-122.64735(3)
	Total					-123.38798(95)
Co(^{4}F)	CISD	-0.5556327	-0.6469961	-0.6915813	-0.7110208	-0.73767(77)
	RCCSD(T)	-0.6143580	-0.7178064	-0.7690287	-0.7912020	-0.8219(11)
	UCCSD(T)	-0.6147478	-0.7182721	-0.7695305	-0.7917233	-0.8225(11)
	CCSDT(Q)	-0.6151622	-0.7184800	-0.76975(*)	-0.79195(*)	-0.8227(11)
	ROHF	-144.3303296	-144.3311368	-144.3312251	-144.3313383	-144.33134(7)
	Total					-145.1541(11)
Ni(^{3}F)	CISD	-0.6105621	-0.7149678	-0.7670986	-0.7899040	-0.82131(93)
	RCCSD(T)	-0.6790395	-0.7964704	-0.8564234	-0.8825722	-0.9189(12)
	UCCSD(T)	-0.6795169	-0.7969812	-0.8569511	-0.8831101	-0.9195(12)
	CCSDT(Q)	-0.6881642	-0.8055330	-0.86614(*)	-0.89258(*)	-0.9295(13)
	ROHF	-168.4614917	-168.4623094	-168.4624643	-168.4625601	-168.46256(4)
	Total					-169.3920(13)
Ni(^{3}D)	CISD	-0.6465397	-0.7570184	-0.8126635	-0.8370597	-0.87068(99)
	RCCSD(T)	-0.7152275	-0.8404277	-0.9054240	-0.9340263	-0.9737(12)
	UCCSD(T)	-0.7153693	-0.8406070	-0.9056235	-0.9342362	-0.9739(12)
	CCSDT(Q)	-0.7150314	-0.8396556	-0.90459(*)	-0.93317(*)	-0.9728(12)
	ROHF	-168.4190995	-168.4200141	-168.4201874	-168.4202614	-168.42026(2)
	Total					-169.3931(12)
Cu(^{2}S)	CISD	-0.6998956	-0.8247607	-0.8882785	-0.9164908	-0.95506(89)
	RCCSD(T)	-0.7738402	-0.9159891	-0.9900301	-1.0231374	-1.06846(99)
	UCCSD(T)	-0.7739280	-0.9160963	-0.9901465	-1.0232562	-1.06859(99)
	CCSDT(Q)	-0.7728824	-0.9141401	-0.98803(*)	-1.02107(*)	-1.0664(10)
	ROHF	-195.3358266	-195.3373699	-195.3373989	-195.3374008	-195.337402(3)
	Total					-196.4038(10)
Zn(^{1}S)	CISD	-0.7139072	-0.8425259	-0.9112300	-0.9413355	-0.9836(15)
	RCCSD(T)	-0.7892886	-0.9339068	-1.0128710	-1.0475878	-1.0964(18)
	UCCSD(T)	-0.7892884	-0.9339071	-1.0128710	-1.0475878	-1.0964(18)
	CCSDT(Q)	-0.7881588	-0.93257(*)	-1.01142(*)	-1.04608(*)	-1.0949(18)
	RHF	-225.2750460	-225.2750619	-225.2750649	-225.2750650	-225.2750654(6)
	Total					-226.3699(18)

Table S8: Atomic kinetic energies [Ha] for the 1st-row elements with ccECPs[He] in D_{2h} point group. aug-cc-pVnZ basis set (cc-pVnZ for Ne).

Atom	Method	DZ	TZ	QZ	5Z	6Z	CBS
H	ROHF	0.49895288	0.49894527	0.49894533	0.49894996		0.498954(2)
He	RHF	2.84397485	2.84397376	2.84398211	2.84397542	2.84397523	
	CISD	2.85517271	2.87995550	2.88332835	2.88469493	2.88512740	2.8855(2)
Li	ROHF	0.076680627	0.07668018	0.07668022	0.076680181		0.07668014(2)
Be	RHF	0.31367034	0.31367174	0.31367101	0.31366632	0.31366995	
	CISD	0.37996620	0.39833731	0.40046822	0.40078321	0.40081561	0.40084(2)
B	ROHF	1.31350447	1.31349404	1.31355496	1.31357391	1.31359811	
	CISD	1.41469876	1.42117834	1.42228561	1.42284300	1.42329158	
	FCI	1.41542556	1.42613474	1.42741224	1.42804175	1.42861274	1.4292(3)
C	ROHF	3.43448649	3.43452459	3.43461006	3.43456695	3.43460019	
	CISD	3.51440134	3.54787465	3.55363577	3.55426728	3.55601079	
	FCI	3.51956182	3.55773078	3.56349068	3.56417396	3.56611336	3.568(1)
N	ROHF	6.82755984	6.82752510	6.82741059	6.82745134	6.82750451	
	CISD	6.86959909	6.94167021	6.95467252	6.95730143	6.95942600	
	FCI	6.88381613	6.95493764	6.96746463	6.97040477	6.9725(*)	6.975(1)
O	ROHF	11.86224486	11.85196677	11.84561055	11.84569222	11.84522573	
	CISD	11.84670197	11.98037873	12.00382205	12.01119666	12.01588644	
	FCI	11.87194641	11.99673997	12.01975665	12.0271(*)	12.0318(*)	12.037(2)
F	ROHF	18.64790112	18.64372752	18.64085665	18.64113790	18.64087260	
	CISD	18.58827042	18.78838611	18.83067241	18.84305889	18.85181858	
	FCI	18.62961103	18.80776779	18.8501(*)	18.8625(*)	18.8713(*)	18.880(4)
Ne	RHF	28.04250304	28.04244770	28.04247300	28.04248372	28.04249187	
	CISD	28.08774862	28.22056329	28.28945965	28.30015252	28.30424228	
	FCI	28.13283740	28.25418488	28.3232(*)	28.3339(*)	28.3380(*)	28.342(2)

Table S9: BFD ECPs kinetic energies [Ha] for selected elements in D_{2h} point group. aug-cc-pVnZ basis set.

Atom	Method	DZ	TZ	QZ	5Z	6Z	CBS
C	ROHF	3.31084033	3.31081800	3.31085129	3.31086049	3.31085102	
	CISD	3.39905497	3.43220003	3.43742568	3.43812989	3.43999849	
	FCI	3.40615847	3.44250862	3.44799624	3.44879717	3.45089891	3.453(1)
N	ROHF	6.75184307	6.75184179	6.75186129	6.75186395	6.75187214	
	CISD	6.80039239	6.87176435	6.88452081	6.88688084	6.88911504	
	FCI	6.81628005	6.88488882	6.89760719	6.90031892	6.902(*)	6.905(1)
O	ROHF	11.62401280	11.61416101	11.60826238	11.60841749	11.60784968	
	CISD	11.61505675	11.75126357	11.77397008	11.78124454	11.78598259	
	FCI	11.64339918	11.76677842	11.78982922	11.797(*)	11.802(*)	11.807(1)
Si	ROHF	1.29873413	1.29867797	1.29868159	1.29868539	1.29868470	
	CISD	1.36205739	1.38173544	1.38679032	1.38739856	1.38826984	
	FCI	1.36884694	1.39511435	1.40164651	1.40249077	1.40355225	1.4046(5)

Table S10: Atomic kinetic energies [Ha] for the 2nd-row elements with ccECPs[Ne] in D_{2h} point group. aug-cc-pVnZ basis set (cc-pVnZ for Ar).

Atom	Method	DZ	TZ	QZ	5Z	6Z	CBS
Na	ROHF	0.08001484	0.07483061	0.07499744	0.07501148		0.07503(1)
Mg	RHF	0.23354968	0.23199509	0.23154500	0.23148284	0.23146504	
	CISD	0.26548027	0.26330003	0.26350512	0.26349267	0.26348253	0.26347(1)
Al	ROHF	0.64171529	0.64170120	0.64171014	0.64171922	0.64170997	
	CISD	0.68754888	0.69602892	0.69844320	0.69924004	0.69942606	
	FCI	0.69123111	0.70218436	0.70489156	0.70584538	0.70606455	0.7063(1)
Si	ROHF	1.32892277	1.32890008	1.32891100	1.32891858	1.32891625	
	CISD	1.38960776	1.40891463	1.41429056	1.41587209	1.41625538	
	FCI	1.39608297	1.42180744	1.42848778	1.43049006	1.43096395	1.4314(2)
P	ROHF	2.35490570	2.35488943	2.35490586	2.35489074	2.35490457	
	CISD	2.42502036	2.45836717	2.46828346	2.47067375	2.47122928	
	FCI	2.43225546	2.47652736	2.48959729	2.4920(*)	2.4926(*)	2.4931(3)
S	ROHF	3.70257242	3.70352986	3.70393876	3.70381590	3.70368510	
	CISD	3.78902994	3.84752777	3.86973265	3.87441933	3.87554308	
	FCI	3.80049085	3.87453980	3.90402772	3.9088(*)	3.9099(*)	3.9110(6)
Cl	ROHF	5.49623725	5.49743938	5.49769904	5.49766709	5.49757874	
	CISD	5.59987572	5.68408507	5.72011850	5.72800838	5.72997729	
	FCI	5.61423106	5.72022458	5.756(*)	5.764(*)	5.766(*)	5.768(1)
Ar	RHF	7.79589481	7.79588297	7.79588540	7.79591613	7.79591535	
	CISD	7.94994979	8.04531135	8.08362249	8.08991031	8.09141320	
	FCI	7.95712773	8.09128251	8.1298(*)	8.1361(*)	8.1376(*)	8.1392(8)

Table S11: Atomic kinetic energies [Ha] for the 2nd-row elements with ccECPs[He] in D_{2h} point group. cc-pCVnZ basis set.

Atom	Method	DZ	TZ	QZ	5Z	6Z	CBS
Na	ROHF	36.52735270	36.52739440	36.52743838	36.52742986	36.52742810	
	CISD	36.56953299	36.71379735	36.73737044	36.74676260	36.75035870	36.754(2)
Mg	RHF	48.55338625	48.55353055	48.55339130	48.55339266	48.55340245	
	CISD	48.72768236	48.76011138	48.77236767	48.78169464	48.78598715	48.790(2)
Al	ROHF	62.89307590	62.89299876	62.89294356	62.89298886	62.89297805	
	CISD	63.02407762	63.11878820	63.14126507	63.15172340	63.15583047	63.160(2)
Si	ROHF	79.41376232	79.41369523	79.41366270	79.41369795	79.41371697	
	CISD	79.56610219	79.67094214	79.69821018	79.70951510	79.71421586	79.719(2)
P	ROHF	98.34763217	98.34753767	98.34753933	98.34759225	98.34755827	
	CISD	98.51183457	98.63625664	98.66838143	98.68140655	98.68736394	98.693(3)
S	ROHF	119.6120740	119.6131095	119.6122989	119.6115298	119.6113622	
	CISD	119.7898780	119.9479402	119.9867627	120.0017791	120.0084628	120.015(3)
Cl	ROHF	144.0484323	144.0498567	144.0492331	144.0486478	144.0484987	
	CISD	144.2370930	144.4315014	144.4786957	144.4966891	144.5051791	144.514(4)
Ar	RHF	170.8576338	170.8574905	170.8574457	170.8574119	170.8575078	
	CISD	171.0530054	171.2817089	171.3365004	171.3576565	171.3683304	171.379(5)

Table S12: Atomic kinetic energies [Ha] for the 3rd-row main group elements with ccECPs in D_{2h} point group. aug-cc-pVnZ basis set (cc-pCVnZ for K, Ca).

Atom	Method	DZ	TZ	QZ	5Z	6Z	CBS
K	ROHF	10.47154301	10.47158948	10.47158031	10.47154409	10.47159990	
	CISD	10.67094386	10.77344574	10.80212489	10.80724403	10.80933057	10.811(1)
Ca	RHF	13.43105715	13.43103412	13.43104385	13.43103436	13.43105075	
	CISD	13.68784850	13.79155454	13.83898979	13.84842237	13.85206945	13.856(2)
Ga	ROHF	0.71683325	0.71680605	0.71680712	0.71680407	0.71680477	
	CISD	0.75469694	0.76107178	0.76307324	0.76351746	0.76378324	
	FCI	0.75756166	0.76513974	0.76717115	0.76768958	0.76797065	0.7683(1)
Ge	ROHF	1.37340615	1.37337458	1.37338602	1.37337603	1.37337625	
	CISD	1.41821943	1.43057985	1.43535297	1.43619257	1.43670066	
	FCI	1.42262816	1.43893523	1.44429303	1.44525263	1.44580878	1.4464(3)
As	ROHF	2.29918816	2.29920741	2.29918168	2.29919531	2.29918832	
	CISD	2.33822054	2.35625126	2.36544329	2.36747993	2.36837897	
	FCI	2.34192027	2.36650052	2.37734101	2.37938(*)	2.38029(*)	2.3812(5)
Se	ROHF	3.28150596	3.28155565	3.28116835	3.28122811	3.28129767	
	CISD	3.32695051	3.36649686	3.38169330	3.38591334	3.38765336	
	FCI	3.33284088	3.38208380	3.40090599	3.40515(*)	3.40689(*)	3.4086(9)
Br	ROHF	4.60159664	4.60264039	4.60262443	4.60262186	4.60267005	
	CISD	4.64630639	4.69963977	4.72990473	4.73726495	4.73992399	
	FCI	4.65339032	4.71876957	4.74915(*)	4.75654(*)	4.75921(*)	4.762(1)
Kr	RHF	6.15676334	6.15659795	6.15681251	6.15675523	6.15681101	
	CISD	6.21644385	6.27728282	6.31615384	6.32677745	6.33038286	
	FCI	6.22657483	6.28751(*)	6.32644(*)	6.33708(*)	6.34069(*)	6.344(2)

Table S13: Atomic kinetic energies [Ha] for the 3rd-row transition elements with ccECPs[Ne] in D_{2h} point group. cc-pCVnZ basis set.

Atom	Method	DZ	TZ	QZ	5Z	CBS
Sc(^{2}D)	ROHF	18.81114626	18.79436449	18.79539726	18.79537922	
	CISD	19.17213606	19.20886255	19.23330475	19.24085720	19.248(4)
Ti(^{3}F)	ROHF	25.88505438	25.86810973	25.86652880	25.86683389	
	CISD	26.21249355	26.27066920	26.28930889	26.30143649	26.314(6)
V(^{4}F)	ROHF	34.54480419	34.54156108	34.54100498	34.54149363	
	CISD	34.94715367	34.98856053	34.98798625	35.00157737	35.015(7)
Cr(^{7}S)	ROHF	46.33993725	46.34630254	46.34615105	46.34601850	
	CISD	46.72814327	46.80257628	46.81694513	46.83905627	46.86(1)
Mn(^{6}S)	ROHF	57.46801485	57.45933930	57.45978807	57.46063830	
	CISD	57.81481658	57.86338258	57.87035748	57.89245175	57.91(1)
Fe(^{5}D)	ROHF	71.87180119	71.85926014	71.85945233	71.86030431	
	CISD	72.25959330	72.29039068	72.28965036	72.31302228	72.34(1)
Co(^{4}F)	ROHF	88.37393133	88.36093093	88.36227973	88.36305363	
	CISD	88.77845411	88.80164715	88.79657950	88.82218324	88.85(1)
Ni(^{3}F)	ROHF	106.9865837	106.9809956	106.9815402	106.9819113	
	CISD	107.4348622	107.4586822	107.4451123	107.4711444	107.50(1)
Ni(^{3}D)	ROHF	108.5309936	108.5416471	108.5394343	108.5392200	
	CISD	109.0852647	109.1300528	109.1067053	109.1307579	109.15(1)
Cu(^{2}S)	ROHF	130.0368644	130.0605199	130.0557909	130.0552440	
	CISD	130.6059338	130.6906066	130.6536798	130.6786121	130.70(1)
Zn(^{1}S)	RHF	150.1003014	150.1018032	150.1016129	150.1016470	
	CISD	150.6015595	150.5955978	150.5631498	150.5899657	150.62(1)

2 Single-determinant FN-DMC energies

This section provides single-determinant FN-DMC energies for ccECP pseudo-atoms. HF nodes in D_{2h} point group with various basis sets are used. The trial wavefunction also includes J_{eI}, J_{ee}, J_{eeI} Jastrow factors. Tables S14-S46 give these data for various elements in selected timesteps. Table S47 gives the FN-DMC energy comparisons with the exact energy for selected TMs. Note that these references are *not* state-averaged references.

Table S14: DMC total energies for He atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-2.90368(7)	-2.90368(6)	-2.90372(5)	-2.90359(7)
0.01	-2.90378(6)	-2.90378(5)	-2.90373(5)	-2.90374(5)
0.005	-2.90373(5)	-2.90372(4)	-2.90376(6)	-2.90369(5)
0.0025	-2.90369(5)	-2.90368(5)	-2.90374(5)	-2.90370(7)
Extrap.	-2.9037206(2)	-2.90374(4)	-2.90375(4)	-2.90374(4)

Table S15: DMC total energies for Be atom with different basis sets.

Timestep	DZ	TZ	QZ
0.02	-1.0082(3)	-1.0086(3)	-1.0087(3)
0.01	-1.0085(3)	-1.0089(3)	-1.0087(3)
0.005	-1.0087(3)	-1.0085(3)	-1.0084(3)
0.0025	-1.0089(2)	-1.0084(2)	-1.0084(2)
Extrap.	-1.0089(2)	-1.0085(2)	-1.0084(2)

Table S16: DMC total energies for B atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-2.6049(1)	-2.60496(9)	-2.60531(9)	-2.60446(8)
0.01	-2.6049(1)	-2.60479(9)	-2.6052(1)	-2.60441(9)
0.005	-2.6045(1)	-2.6047(1)	-2.6048(1)	-2.60438(9)
0.0025	-2.6052(1)	-2.60455(9)	-2.60490(9)	-2.60439(8)
0.001	-2.60464(9)	-2.60449(9)	-2.6049(1)	-2.6043(1)
Extrap.	-2.6047(2)	-2.60452(4)	-2.60481(7)	-2.60436(1)

Table S17: DMC Total energies for C atom with different basis

Timestep	DZ	TZ	QZ	5Z	6Z
0.02	-5.4055(1)	-5.4058(1)	-5.4057(1)	-5.4058(1)	-5.4060(1)
0.01	-5.4055(1)	-5.4050(1)	-5.4050(1)	-5.4050(1)	-5.4055(1)
0.0075	-5.4049(1)	-5.4049(1)	-5.4050(1)	-5.4049(1)	-5.4052(1)
0.005	-5.4050(1)	-5.4050(1)	-5.4048(1)	-5.4047(1)	-5.4050(1)
Extrap.	-5.4049(3)	-5.4046(1)	-5.4045(1)	-5.40432(3)	-5.4047(1)

Table S18: DMC total energies for N atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-9.7535(1)	-9.7543(1)	-9.7541(1)	-9.7539(1)
0.01	-9.7538(1)	-9.7541(1)	-9.7540(1)	-9.7540(1)
0.005	-9.7536(1)	-9.7545(1)	-9.7539(1)	-9.7541(1)
0.0025	-9.7536(1)	-9.7540(1)	-9.7538(1)	-9.7539(1)
0.001	-9.7536(1)	-9.7540(1)	-9.7538(1)	-9.7538(1)
Extrap.	-9.75363(8)	-9.7541(1)	-9.75381(2)	-9.75391(9)

Table S19: DMC total energies for O atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-15.8702(2)	-15.8730(2)	-15.8698(1)	-15.8708(1)
0.01	-15.8698(2)	-15.8713(2)	-15.8694(2)	-15.8696(1)
0.005	-15.8697(1)	-15.8701(2)	-15.8697(1)	-15.8695(1)
0.0025	-15.8694(1)	-15.8694(2)	-15.8691(1)	-15.8695(1)
0.001	-15.8695(1)	-15.8695(2)	-15.8689(1)	-15.8690(2)
Extrap.	-15.86942(6)	-15.8691(1)	-15.8691(2)	-15.8691(2)

Table S20: DMC total energies for F atom with different basis sets.

Timestep	DZ	TZ	QZ
0.02	-24.1858(4)	-24.1860(3)	-24.1854(4)
0.01	-24.1839(3)	-24.1835(3)	-24.1840(2)
0.005	-24.1825(2)	-24.1828(3)	-24.1830(2)
0.0025	-24.1820(2)	-24.1823(2)	-24.1821(3)
Extrap.	-24.1815(2)	-24.1818(2)	-24.1820(2)

Table S21: DMC total energies for Ne atom with different basis sets.

Timestep	DZ	TZ	QZ
0.02	-35.0255(4)	-35.0253(4)	-35.0255(5)
0.01	-35.0232(3)	-35.0227(3)	-35.0232(3)
0.005	-35.0223(3)	-35.0220(2)	-35.0219(3)
0.0025	-35.0214(3)	-35.0215(3)	-35.0214(3)
Extrap.	-35.0210(2)	-35.0209(2)	-35.0207(2)

Table S22: DMC total energies for Mg atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-0.82309(3)	-0.82306(3)	-0.82309(3)	-0.82307(3)
0.01	-0.82296(3)	-0.82308(3)	-0.82306(3)	-0.82306(3)
0.005	-0.82300(4)	-0.82317(3)	-0.82309(3)	-0.82300(3)
0.0025	-0.82303(3)	-0.82308(3)	-0.82302(3)	-0.82312(3)
0.001	-0.82303(3)	-0.82307(3)	-0.82309(3)	-0.82298(3)
Extrap.	-0.82300(3)	-0.82310(3)	-0.82306(2)	-0.82302(4)

Table S23: DMC total energies for Al atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-1.93600(6)	-1.93559(7)	-1.93567(7)	-1.93587(6)
0.01	-1.93583(6)	-1.93563(6)	-1.93584(7)	-1.93586(6)
0.005	-1.93612(6)	-1.93558(6)	-1.93562(6)	-1.93584(7)
0.0025	-1.93587(6)	-1.93553(6)	-1.93570(6)	-1.93588(6)
0.001	-1.93599(6)	-1.93574(6)	-1.93589(6)	-1.93597(6)
Extrap.	-1.93595(9)	-1.93563(6)	-1.93579(9)	-1.93591(3)

Table S24: DMC total energies for Si atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-3.75897(7)	-3.75934(8)	-3.75895(8)	-3.75918(7)
0.01	-3.75902(7)	-3.75911(7)	-3.75894(7)	-3.75914(7)
0.005	-3.75902(8)	-3.75933(8)	-3.75905(8)	-3.75914(8)
0.0025	-3.75895(8)	-3.75920(7)	-3.75893(8)	-3.75914(8)
0.001	-3.75907(8)	-3.75913(8)	-3.75876(7)	-3.75914(8)
Extrap.	-3.75903(3)	-3.75917(7)	-3.75888(8)	-3.759131(5)

Table S25: DMC total energies for P atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-6.45627(9)	-6.45611(9)	-6.45609(9)	-6.45641(9)
0.01	-6.4563(1)	-6.45622(8)	-6.4561(1)	-6.45640(9)
0.005	-6.45642(9)	-6.45641(9)	-6.45610(8)	-6.45659(9)
0.0025	-6.45647(9)	-6.4561(1)	-6.45632(9)	-6.4562(1)
0.001	-6.45647(9)	-6.45629(9)	-6.4562(1)	-6.45656(9)
Extrap.	-6.45648(1)	-6.4563(1)	-6.45624(6)	-6.4565(1)

Table S26: DMC total energies for S atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-10.0905(1)	-10.0904(1)	-10.0901(1)	-10.0901(1)
0.01	-10.0906(1)	-10.0903(1)	-10.0903(1)	-10.0903(1)
0.005	-10.0906(1)	-10.0905(1)	-10.0903(1)	-10.0903(1)
0.0025	-10.0907(1)	-10.0905(1)	-10.0905(1)	-10.0902(1)
0.001	-10.0907(1)	-10.0904(1)	-10.0905(1)	-10.0901(1)
Extrap.	-10.09066(3)	-10.09046(6)	-10.09050(4)	-10.09023(8)

Table S27: DMC total energies for Cl atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-14.9178(2)	-14.9171(1)	-14.9172(2)	-14.9175(1)
0.01	-14.9181(1)	-14.9175(1)	-14.9173(2)	-14.9167(1)
0.005	-14.9179(1)	-14.9175(1)	-14.9173(2)	-14.9172(1)
0.0025	-14.9176(1)	-14.9175(1)	-14.9176(2)	-14.9173(1)
0.001	-14.9179(2)	-14.9171(1)	-14.9177(1)	-14.9176(1)
Extrap.	-14.9178(1)	-14.9174(2)	-14.91759(7)	-14.9173(3)

Table S28: DMC total energies for Ar atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-21.0615(2)	-21.0617(2)	-21.0614(2)	-21.0615(2)
0.01	-21.0613(2)	-21.0615(2)	-21.0616(1)	-21.0616(2)
0.005	-21.0615(2)	-21.0616(2)	-21.0615(2)	-21.0618(2)
0.0025	-21.0615(2)	-21.0615(2)	-21.0618(2)	-21.0617(2)
0.001	-21.0611(2)	-21.0613(2)	-21.0615(2)	-21.0618(2)
Extrap.	-21.0613(1)	-21.06141(7)	-21.0617(1)	-21.06177(5)

Table S29: DMC total energies for K atom with different basis sets.

Timestep	DZ	TZ	QZ
0.02	-28.2401(3)	-28.2398(4)	-28.2398(4)
0.01	-28.2395(3)	-28.2399(3)	-28.2397(3)
0.005	-28.2395(3)	-28.2394(3)	-28.2392(3)
0.0025	-28.2393(2)	-28.2393(2)	-28.2395(2)
Extrap.	-28.2393(2)	-28.2393(2)	-28.2393(2)

Table S30: DMC total energies for Ca atom with different basis sets.

Timestep	DZ	TZ	QZ
0.02	-36.7069(4)	-36.7069(6)	-36.7058(5)
0.01	-36.7057(4)	-36.7054(3)	-36.7058(4)
0.005	-36.7049(4)	-36.7056(3)	-36.7057(3)
0.0025	-36.7056(4)	-36.7049(3)	-36.7051(3)
Extrap.	-36.7047(3)	-36.7049(3)	-36.7054(2)

Table S31: DMC total energies for Sc atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-46.5227(5)	-46.5238(5)	-46.5228(5)	-46.5232(5)
0.01	-46.5211(5)	-46.5213(4)	-46.5200(5)	-46.5221(4)
0.005	-46.5205(5)	-46.5211(5)	-46.5214(4)	-46.5205(5)
0.0025	-46.5204(5)	-46.5194(5)	-46.5199(5)	-46.5202(4)
0.001	-46.5190(4)	-46.5201(4)	-46.5193(4)	-46.5197(4)
Extrap.	-46.5193(3)	-46.5196(3)	-46.5195(6)	-46.5197(3)

Table S32: DMC total energies for Ti atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-58.0538(5)	-58.0535(6)	-58.0530(6)	-58.0518(5)
0.01	-58.0483(5)	-58.0481(6)	-58.0484(6)	-58.0481(5)
0.005	-58.0461(5)	-58.0469(5)	-58.0463(5)	-58.0468(5)
0.0025	-58.0464(5)	-58.0463(5)	-58.0458(6)	-58.0458(5)
0.001	-58.0453(4)	-58.0458(5)	-58.0458(5)	-58.0453(6)
Extrap.	-58.0446(5)	-58.0451(4)	-58.0448(4)	-58.0450(1)

Table S33: DMC total energies for V atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-71.3831(5)	-71.3826(6)	-71.3830(7)	-71.3834(6)
0.01	-71.3780(6)	-71.3780(6)	-71.3781(6)	-71.3785(6)
0.005	-71.3758(6)	-71.3772(5)	-71.3742(7)	-71.3765(7)
0.0025	-71.3734(6)	-71.3734(4)	-71.3748(5)	-71.3736(6)
0.001	-71.3756(4)	-71.3738(4)	-71.3727(6)	-71.3741(5)
Extrap.	-71.3740(8)	-71.3732(7)	-71.3728(5)	-71.3733(5)

Table S34: DMC total energies for Cr atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-86.5976(6)	-86.5992(6)	-86.5987(7)	-86.6003(7)
0.01	-86.5927(6)	-86.5935(5)	-86.5929(6)	-86.5943(6)
0.005	-86.5893(5)	-86.5900(5)	-86.5900(6)	-86.5914(6)
0.0025	-86.5857(5)	-86.5890(6)	-86.5885(7)	-86.5874(5)
0.001	-86.5852(6)	-86.5875(6)	-86.5869(5)	-86.5873(6)
Extrap.	-86.5850(7)	-86.5871(2)	-86.5866(2)	-86.5867(7)

Table S35: DMC total energies for Mn atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-103.8390(7)	-103.8403(7)	-103.8422(7)	-103.8415(8)
0.01	-103.8336(6)	-103.8335(7)	-103.8340(7)	-103.8330(8)
0.005	-103.8301(7)	-103.8314(6)	-103.8290(6)	-103.8296(5)
0.0025	-103.8287(7)	-103.8259(6)	-103.8282(6)	-103.8264(6)
0.001	-103.8257(6)	-103.8251(5)	-103.8254(6)	-103.8250(5)
Extrap.	-103.8263(7)	-103.825(1)	-103.8251(5)	-103.8246(4)

Table S36: DMC total energies for Fe atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-123.3241(8)	-123.3298(7)	-123.3294(8)	-123.3289(7)
0.01	-123.3181(7)	-123.3199(6)	-123.3196(7)	-123.3188(7)
0.005	-123.3146(6)	-123.3143(6)	-123.3140(7)	-123.3152(6)
0.0025	-123.3118(5)	-123.3118(7)	-123.3109(8)	-123.3118(7)
0.001	-123.3102(6)	-123.3106(7)	-123.3099(7)	-123.3105(7)
Extrap.	-123.3102(5)	-123.3094(2)	-123.3087(2)	-123.3098(4)

Table S37: DMC total energies for Co atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-145.0906(7)	-145.0913(8)	-145.0923(8)	-145.0933(9)
0.01	-145.0791(7)	-145.0810(8)	-145.0808(7)	-145.0799(7)
0.005	-145.0758(7)	-145.0758(8)	-145.0759(7)	-145.0746(7)
0.0025	-145.0720(7)	-145.0717(6)	-145.0736(7)	-145.0714(6)
0.001	-145.0703(8)	-145.0699(5)	-145.0702(7)	-145.0731(6)
Extrap.	-145.0695(5)	-145.0691(4)	-145.0700(5)	-145.070(1)

Table S38: DMC total energies for Ni (^3F) atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-169.3132(8)	-169.313(1)	-169.3131(8)	-169.3145(6)
0.01	-169.3014(8)	-169.3002(8)	-169.3024(8)	-169.3006(9)
0.005	-169.2934(9)	-169.2941(6)	-169.2961(5)	-169.2957(7)
0.0025	-169.2893(8)	-169.2909(7)	-169.2911(6)	-169.2921(7)
0.001	-169.2894(7)	-169.2882(7)	-169.2876(6)	-169.2888(8)
Extrap.	-169.2874(7)	-169.2874(2)	-169.288(1)	-169.2885(5)

Table S39: DMC total energies for Cu atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-196.343(1)	-196.3417(7)	-196.3422(9)	-196.3442(8)
0.01	-196.3287(8)	-196.330(1)	-196.3313(8)	-196.3291(7)
0.005	-196.3221(8)	-196.3241(7)	-196.3236(7)	-196.3217(8)
0.0025	-196.3174(9)	-196.3189(8)	-196.3174(7)	-196.3198(9)
0.001	-196.3149(8)	-196.3165(7)	-196.3173(7)	-196.3188(7)
Extrap.	-196.3139(4)	-196.3161(7)	-196.316(1)	-196.3163(8)

Table S40: DMC total energies for Zn atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-226.3043(8)	-226.3047(9)	-226.3069(7)	-226.3049(9)
0.01	-226.2893(8)	-226.2894(8)	-226.2890(7)	-226.2892(8)
0.005	-226.2833(7)	-226.2848(7)	-226.2830(7)	-226.2829(7)
0.0025	-226.2795(6)	-226.2798(8)	-226.2789(7)	-226.2772(8)
0.001	-226.2763(6)	-226.2774(8)	-226.2762(7)	-226.2762(7)
Extrap.	-226.2756(4)	-226.2765(7)	-226.2746(7)	-226.2743(6)

Table S41: DMC total energies for Ga atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-2.0390(2)	-2.0387(2)	-2.0386(2)	-2.0386(4)
0.01	-2.0393(2)	-2.0388(2)	-2.0393(2)	-2.0386(2)
0.005	-2.0388(2)	-2.0389(2)	-2.0389(2)	-2.0388(2)
0.0025	-2.0390(2)	-2.0387(2)	-2.0390(2)	-2.0391(2)
Extrap.	-2.0389(2)	-2.0388(2)	-2.0392(2)	-2.0390(2)

Table S42: DMC total energies for Ge atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-3.7418(4)	-3.7414(3)	-3.7420(4)	-3.7424(4)
0.01	-3.7421(3)	-3.7419(3)	-3.7421(3)	-3.7425(5)
0.005	-3.7423(3)	-3.7422(3)	-3.7421(3)	-3.7426(3)
0.0025	-3.7431(4)	-3.7429(3)	-3.7429(3)	-3.7427(2)
Extrap.	-3.7429(3)	-3.7429(3)	-3.7426(3)	-3.7427(2)

Table S43: DMC total energies for As atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-6.1625(2)	-6.1617(2)	-6.1625(3)	-6.1617(2)
0.01	-6.1630(2)	-6.1625(3)	-6.1627(2)	-6.1628(2)
0.005	-6.1625(2)	-6.1634(3)	-6.1629(3)	-6.1633(2)
0.0025	-6.1630(2)	-6.1632(2)	-6.1632(2)	-6.1629(2)
Extrap.	-6.1629(2)	-6.1637(2)	-6.1632(2)	-6.1635(2)

Table S44: DMC total energies for Se atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-9.2964(1)	-9.2966(2)	-9.2964(1)	-9.2965(1)
0.01	-9.2967(1)	-9.2964(2)	-9.2963(1)	-9.2964(1)
0.005	-9.2965(1)	-9.2964(2)	-9.2963(1)	-9.2962(1)
0.0025	-9.2965(1)	-9.2967(2)	-9.2966(1)	-9.2964(1)
Extrap.	-9.2966(1)	-9.2965(1)	-9.2965(1)	-9.2963(1)

Table S45: DMC total energies for Br atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-13.3133(1)	-13.3134(1)	-13.3133(1)	-13.3134(1)
0.01	-13.3136(1)	-13.3135(1)	-13.3134(1)	-13.3134(1)
0.005	-13.3136(1)	-13.3134(1)	-13.3133(1)	-13.3133(1)
0.0025	-13.3137(1)	-13.3133(1)	-13.3133(1)	-13.3134(1)
Extrap.	-13.3138(1)	-13.3133(1)	-13.3133(1)	-13.3133(1)

Table S46: DMC total energies for Kr atom with different basis sets.

Timestep	DZ	TZ	QZ	5Z
0.02	-18.4679(1)	-18.4679(1)	-18.4684(1)	-18.4679(1)
0.01	-18.4680(1)	-18.4681(1)	-18.4679(1)	-18.4679(1)
0.005	-18.4681(1)	-18.4678(1)	-18.4678(1)	-18.4678(1)
0.0025	-18.4678(1)	-18.4678(1)	-18.4678(1)	-18.4679(1)
Extrap.	-18.4679(1)	-18.4678(1)	-18.4675(1)	-18.4680(1)

Table S47: DMC energy comparisons for selected atoms. HF nodes are used obtained at D_{2h} point group. DMC calculations use $\tau = (0.02, 0.01, 0.005, 0.0025)$ Ha^{-1} timestep extrapolation. Here, $\eta = (100\epsilon)/|E_{corr}|$ where ϵ represents the total DMC error, namely, combined fixed-node and localization biases.

Atom	State	"Exact"(Ha)	DMC/HF(Ha)	ϵ(mHa)	η
Ti	(^{3}F)	-58.09263(76)	-58.0450(3)	47.6(8)	9.8(2)
V	(^{4}F)	-71.44178(59)	-71.3730(2)	68.8(6)	12.6(1)
Co	(^{4}F)	-145.1541(10)	-145.0711(3)	83(1)	10.0(1)
Ni	(^{3}F)	-169.3912(12)	-169.2894(3)	102(1)	11.1(1)
Ni	(^{3}D)	-169.3932(12)	-169.3075(3)	86(1)	8.8(1)

3 Multi-determinant FN-DMC energies

This section provides multi-determinant fixed-node DMC energies for selected ccECP pseudoatoms. For Be, B, and C we employ two-configuration nodes obtained from CASSCF with $(2s, 2p)$ active space. Tables S48 and S49 give the data for these elements. All trial wavefunctions also include J_{eI}, J_{ee}, J_{eeI} Jastrow factors.

Table S50 provides energies for CIPSI vs DMC methods. Table S51 provides data for various ECPs as a demonstration of CIPSI convergence.

Table S48: Two-configuration QMC energies for selected atoms. DMC results are from $\tau = (0.02, 0.01, 0.005, 0.0025)$ Ha^{-1} time step extrapolations. D represents the determinantal part while J represents the Jastrow factor. All values are in Ha.

Atom	VMC(D)	VMC(DJ)	DMC
Be	-1.00789(5)	-1.00881(6)	-1.0100(2)
B	-2.5765(2)	-2.6043(2)	-2.6107(4)
C	-5.3349(3)	-5.4014(2)	-5.4086(2)

Table S49: Two-configuration QMC energy comparisons for selected atoms. DMC results are estimated from $\tau = (0.02, 0.01, 0.005, 0.0025)$ Ha^{-1} time step extrapolations. Here, $\eta = (100\epsilon)/|E_{corr}|$ where ϵ represents the total DMC error, namely, the combination of fixed-node and localization biases.

Atom	"Exact"(Ha)	DMC(Ha)	ϵ(mHa)	η
Be	-1.01023896(12)	-1.0100(2)	0.2(2)	0.5(4)
B	-2.61531(13)	-2.6107(4)	4.6(4)	6.1(6)
C	-5.41753(31)	-5.4086(2)	8.9(4)	8.6(4)

Table S50: Comparison of total energies using different methods and basis sets (cc-pVnZ) for F atom with ccECP[He] (data for Fig. 1 in the main paper). HF reference was used for CIPSI expansions. FN-DMC is extrapolated with $\tau = (0.01, 0.005, 0.0025)$ Ha^{-1} time steps and Jastrow factor was not included.

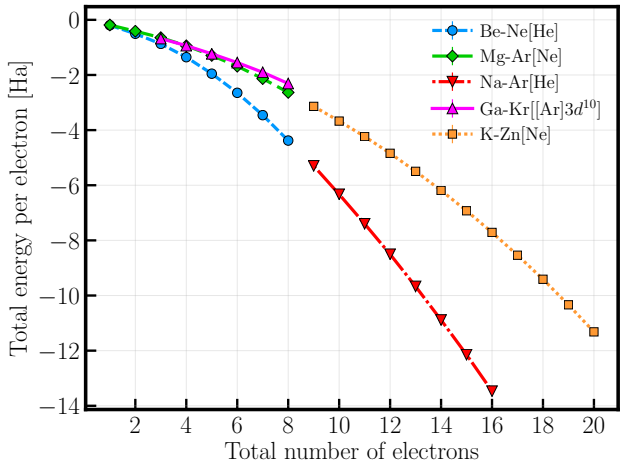
Basis	# Dets.	E(var)	E+PT2	DMC
DZ	1	-23.93640517	-24.10991495	-24.17037(67)
	22	-23.99389045	-24.09304827	-24.16353(49)
	124	-24.07182532	-24.08646612	-24.17512(40)
	1812	-24.08547306	-24.08608680	-24.18061(57)
	10541	-24.08585222	-24.08607544	-24.18098(81)
TZ	1	-23.93760798	-24.18780289	-24.16974(56)
	12	-23.96499018	-24.17884623	-24.16924(52)
	157	-24.06565653	-24.16089033	-24.17463(49)
	1243	-24.14796428	-24.15897770	-24.18726(55)
	18210	-24.15693387	-24.15870476	-24.18935(71)
	150284	-24.15829091	-24.15868605	-24.1920(11)
QZ	1	-23.93782653	-24.21082191	-24.17021(57)
	14	-23.96321873	-24.20217212	-24.16913(60)
	134	-24.03003434	-24.18905589	-24.17045(58)
	1670	-24.15135399	-24.18202990	-24.18686(53)
	11442	-24.17628321	-24.18207832	-24.19397(62)
	118854	-24.18042552	-24.18204947	-24.19491(82)

4 Energies per electron

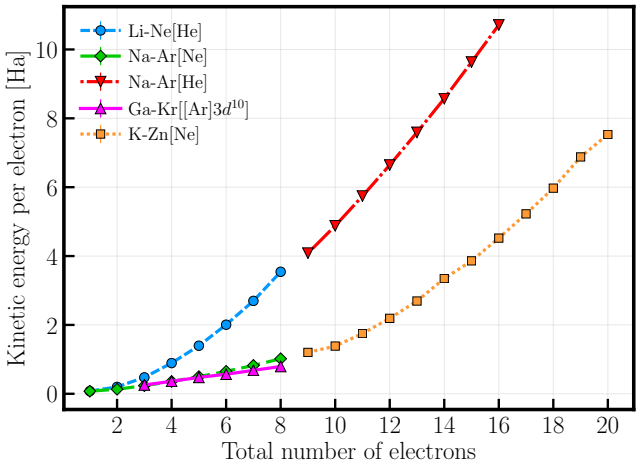
Figures S1a and S1b plot the total and kinetic energies per electron, respectively, for all considered ccECP pseudoatoms.

Table S51: Comparison of F atom CIPSI energies for ccECP, BFD, and eCEPP.

ECP	cc-pVDZ			cc-pVTZ			cc-pVQZ		
	# Dets.	E(var)	E+PT2	# Dets.	E(var)	E+PT2	# Dets.	E(var)	E+PT2
	1	-23.936405	-24.109915	1	-23.937608	-24.187803	1	-23.937827	-24.210822
	2	-23.946244	-24.105803	4	-23.945130	-24.185023	4	-23.943182	-24.208629
	6	-23.964866	-24.098356	9	-23.960097	-24.179539	7	-23.952521	-24.205347
	22	-23.993890	-24.093048	24	-23.979285	-24.174556	17	-23.966651	-24.201345
	64	-24.037202	-24.088332	67	-24.017163	-24.168348	42	-23.988364	-24.195238
ccECP	124	-24.071825	-24.086466	157	-24.065657	-24.160890	134	-24.030034	-24.189056
	258	-24.082848	-24.086302	365	-24.106130	-24.159095	290	-24.080455	-24.183395
	740	-24.084809	-24.086124	891	-24.139887	-24.158960	677	-24.118162	-24.182366
	2333	-24.085572	-24.086085	1911	-24.151931	-24.158935	1711	-24.152144	-24.182035
	5713	-24.085851	-24.086076	5955	-24.155096	-24.158759	4003	-24.170274	-24.182173
	10541	-24.085852	-24.086075	18210	-24.156934	-24.158705	11442	-24.176283	-24.182080
				60965	-24.158055	-24.158689	35369	-24.178730	-24.182057
				150284	-24.158291	-24.158686	118854	-24.180426	-24.182049
	# Dets.	E(var)	E+PT2	# Dets.	E(var)	E+PT2	# Dets.	E(var)	E+PT2
	1	-23.937011	-24.118130	1	-23.938216	-24.193552	1	-23.938435	-24.215864
	2	-23.946891	-24.113845	4	-23.945720	-24.190775	4	-23.943793	-24.213648
	6	-23.965582	-24.106022	9	-23.960740	-24.185108	7	-23.953154	-24.210278
	22	-23.994678	-24.100227	34	-23.986017	-24.178900	17	-23.967306	-24.206201
	64	-24.042137	-24.094969	76	-24.029355	-24.171347	49	-23.991227	-24.199570
	120	-24.076899	-24.093120	211	-24.082860	-24.165042	151	-24.036669	-24.192751
BFD	254	-24.088733	-24.092988	475	-24.122166	-24.163839	332	-24.088804	-24.187128
	740	-24.091308	-24.092782	1087	-24.149963	-24.163847	708	-24.124888	-24.186518
	2284	-24.092175	-24.092727	2749	-24.157719	-24.163756	1780	-24.157287	-24.186203
	5092	-24.092517	-24.092715	8739	-24.160487	-24.163609	4136	-24.174398	-24.186312
	12542	-24.092540	-24.092714	27643	-24.162203	-24.163571	11745	-24.180335	-24.186192
				83211	-24.163040	-24.163558	37090	-24.182827	-24.186165
				128164	-24.163127	-24.163568	125107	-24.184548	-24.186150
	# Dets.	E(var)	E+PT2	# Dets.	E(var)	E+PT2	# Dets.	E(var)	E+PT2
	1	-23.890536	-24.066367	1	-23.891632	-24.143132	1	-23.891880	-24.165073
	2	-23.900514	-24.062016	2	-23.897008	-24.140836	4	-23.897156	-24.162914
	6	-23.919361	-24.054200	6	-23.909645	-24.135776	7	-23.907024	-24.159381
	22	-23.948558	-24.048792	22	-23.928561	-24.130915	17	-23.920974	-24.155464
	64	-23.992191	-24.044018	64	-23.967693	-24.123849	45	-23.945821	-24.147785
	124	-24.026979	-24.042118	157	-24.019437	-24.115852	147	-23.989325	-24.142023
eCEPP	258	-24.038071	-24.041949	385	-24.061684	-24.113959	329	-24.040059	-24.136817
	741	-24.040295	-24.041732	887	-24.094906	-24.113803	731	-24.075151	-24.136223
	2289	-24.041138	-24.041683	1883	-24.106590	-24.113743	1843	-24.107942	-24.135943
	5024	-24.041451	-24.041673	5798	-24.109813	-24.113555	4108	-24.124531	-24.136086
	11960	-24.041476	-24.041672	17774	-24.111672	-24.113496	11594	-24.130282	-24.135972
				59281	-24.112818	-24.113480	36461	-24.132667	-24.135942
				132983	-24.113073	-24.113490	123611	-24.134347	-24.135940



(a) Total energies per electron for ccECPs.



(b) Kinetic energies per electron for ccECPs.

Figure S1