

Supplementary data

Contents

Table S1 Harmonic frequencies from atomic spring constants for the ground states of alkali-metal diatomic molecules.

Table S2 Harmonic frequencies for the $a^3\Sigma^+/a^3\Sigma_u^+$, $b^3\Pi/b^3\Pi_u$, and $A^1\Sigma^+/A^1\Sigma_u^+$ excited states of alkali-metal diatomic molecules.

Table S3 Harmonic frequencies from the $AB\{AX+BY-XY\}$ and $AB\{A_2+BC-C_2\}$ schemes for some sets of the ground-state molecules.

Section S1 Results for molecules from groups IIA & VIA.

Table S4 Harmonic frequencies obtained from theory of atomic spring constants for the $X^1\Sigma^+$ states of BeO, BeS, MgO, MgS, CaO, CaS, SrO, SrS, BaO, and BaS.

Figure S1 Total electronic densities in the ground states of (a). Li_2 ; (b). LiNa; and (c). LiK molecules. The data are calculated using the *Gaussian 03* package⁷³ at Hartree-Fock/6-311++g(3df,3dp) level. Parameters are the same for different molecules. Resolution=0.1 Å and full density matrixex are used.

Figure S2 Errors from the $AB\{AX+BY-XY\}$ schemes with $(n_B-n_X)\times(n_A-n_Y)=-1$. All the errors are less than zero in this figure.

Figure S3 Errors from the $AB\{AX+BY-XY\}$ schemes with $(n_B-n_X)\times(n_A-n_Y)=1$. All the errors are greater than zero in this figure.

Figure S4 Total electronic densities in the ground states of molecules in (a) {BH, SiH, BF, SiF} and (b) {LiO, LiCl, NaO, NaCl} sets: (a1) BF; (a2) BH; (a3) SiF; (a4) SiH; (b1) NaCl; (b2) LiCl; (b3) NaO; (b4) LiO. The data are calculated using the *Gaussian 03* package⁷³ at B3LYP/6-311++g(3df,3dp) level. Resolution=0.1 Å. Parameters are the same for different molecules. Full density matrixes are used.

Section S2 Results for group IB molecules

Figure S5 Errors for AuCu, AgCu, and AgAu from molecules of group IB atoms and their hydrides

Table S1. Harmonic frequencies from atomic spring constants for the ground states of alkali-metal diatomic molecules. The isotope species are ^7Li , ^{23}Na , ^{39}K , ^{85}Rb , and ^{133}Cs in the molecules.

	Experiments		Present work			<i>Ab initio</i>		
	ω_e/cm^{-1}	Ref.	ω_e/cm^{-1}	Scheme	$\delta\omega_e/\text{cm}^{-1}$	ω_e/cm^{-1}	$\delta\omega_e/\text{cm}^{-1}$	Ref.
Li_2	351.4066	23	358.6788	{LiNa-Na ₂ }	7.2722			
Na_2	159.0855	23	161.2740	{LiNa-Li ₂ }	2.1885			
LiNa	256.5412	23	254.4643	{Li ₂ +Na ₂ }	-2.0769			
LiK	212.0386	27	213.039	{LiRb+NaK-NaRb}	1.0004	210.9	-1.14	49
						219.8	7.76	27
						195.0	-0.18	53
LiRb	195.1839	28	195.8958	{LiCs+NaRb-NaCs}	0.7118	194.0	-1.18	57
						194.3449	{LiK+RbNa-Kna}	-0.8391
LiCs	184.6989	29	184.0851	{LiRb+NaCs-NaRb}	-0.6138	187.1	2.4	52
NaK	124.0229	30	123.5423	{NaRb+LiK-LiRb}	-0.4806	123.44	-0.58	18
NaRb	106.856	31	106.5332	{NaCs+LiRb-LiCs}	-0.3228	103.9	-2.96	57
			107.2450	{NaK+RbLi-Kli}	0.3890	106.0	-0.86	53
NaCs	98.87866	32	99.15821	{NaRb+LiCs-LiRb}	0.2795	99.97	0.09	52
K_2	92.4	25	92.75748	{KRb-Rb ₂ }	0.3575	93.18	1.22	18
			92.7681	{KRb*-Rb ₂ }	0.3681	91.80	-0.60	49
KRb	75.8418	33	75.7074	{K ₂ +Rb ₂ }	-0.1344	76	0.16	59
			75.84577*	69	76.1234	{RbCs+K ₂ -Cs ₂ }	0.2816	76.3
			76.36					0.52
KCs	68.394	34	68.0233	{KRb+RbCs-Rb ₂ }	-0.3707	69.21	0.82	52
			68.6678	{Cs ₂ +NaK-Na ₂ }	0.2738	68.7	0.31	55
			67.5804	{Cs ₂ +K ₂ }	-0.8136	69.9	1.51	58
			68.0265	{KRb*+RbCs-Rb ₂ }	-0.3675	67.2	-1.19	55
Rb ₂	57.78916	26	57.97958	{KRb-K ₂ }	0.1904	59	1.21	50
			57.47408	{KRb+RbCs-KCs}	-0.3151			
			57.47683	{KRb*+RbCs-KCs}	-0.3123			
RbCs	50.01374	35	49.78458	{Rb ₂ +Cs ₂ }	-0.2292	51.35	1.34	56
			50.26695	{Rb ₂ +KCs-KRb}	0.2532			
			49.8587	{Cs ₂ +KRb-K ₂ }	-0.1550			
			49.8609	{Cs ₂ +KRb*-K ₂ }	-0.1529			
			50.26471	{Rb ₂ +KCs-KRb*}	0.2510			
Cs_2	42.022	24	42.37754	{RbCs-Rb ₂ }	0.3555			

* ω_e from ref.69.

Table S2. Harmonic frequencies for the $a^3\Sigma^+/a^3\Sigma_u^+$, $b^3\Pi/b^3\Pi_u$, and $A^1\Sigma^+/A^1\Sigma_u^+$ excited states of alkali-metal diatomic molecules. The isotope species are ^7Li , ^{23}Na , ^{39}K , ^{85}Rb , and ^{133}Cs in the molecules.

$a^3\Sigma_u^+$	Experiments		Present	Work	Scheme	<i>ab initio</i>		
	ω_e/cm^{-1}	Refs	ω_e/cm^{-1}	$\delta\omega_e/\text{cm}^{-1}$		ω_e/cm^{-1}	$\delta\omega_e/\text{cm}^{-1}$	Refs
Li_2	65.13	36						
Na_2	24.15	36	23.8939	-0.2561	{NaK-K ₂ }			
K_2	21.7123537	37	21.3988	-0.3135	{NaK-Na ₂ }	20.81	-0.90	18
			22.1035	0.3912	{KCs-Cs ₂ }	21.61(exp)	-0.10	71
Cs_2	11.6336	38	11.8387	0.2051	{KCs-K ₂ }			
$a^3\Sigma^+$								
LiK	44.2(±1.5)	39	43.3148	-0.8852	{Li ₂ +NaK-Na ₂ }			
			43.7083	-0.4917	{Li ₂ +K ₂ }			
			44.1903	-0.0097	{Li ₂ +KCs-Cs ₂ }			
LiRb	40.13(theor.)	51	38.7381	-1.3919	{Li ₂ +KRb*-K ₂ }	41.2	1.07	57
NaK	23.0099	40	22.1769	-0.8330	{NaRb+K ₂ -KRb*}			
			23.1528	0.1429	{Na ₂ +K ₂ }	22.65	-0.36	18
			23.3261	0.3162	{Na ₂ +KCs-Cs ₂ }	22.63	-0.38	72
NaRb	18.859	41	19.7156	0.8566	{Na ₂ +KRb*-NaK}	15.3	-3.56	57
			19.4965	0.6375	{NaK+KRb*-K ₂ }			
			19.6051	0.7461	{Na ₂ +KRb*-K ₂ }			
KRb	17.4(theor.)	54	16.7367	-0.6633	{K ₂ +NaRb-NaK}			
			17.9151	0.5151	{K ₂ +LiRb*-Li ₂ }			
KCs	17.52	34	17.3673	-0.1527	{K ₂ +Cs ₂ }	17.6	0.08	55
			17.2418	-0.2782	{Cs ₂ +NaK-Na ₂ }	16.5	-1.02	58
						16.0	-1.52	55
						15.91	-1.61	52

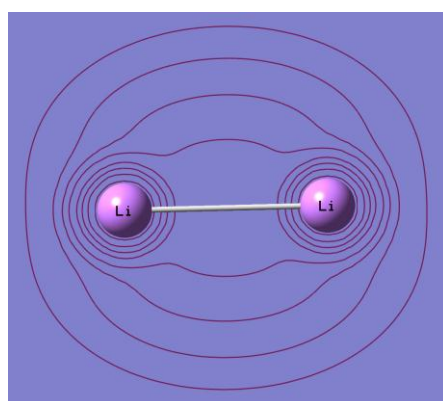
* ω_e from theoretical results: LiRb(Ref. 51); KRb(Ref.54).

Table S2. continued.

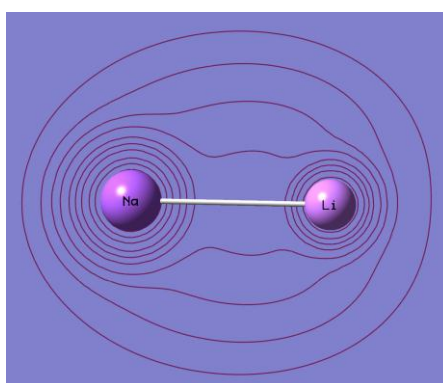
$b^3\Pi_u$	Experiments		Present work			<i>ab initio</i>		
	ω_e/cm^{-1}	Ref	ω_e/cm^{-1}	$\delta\omega_e/\text{cm}^{-1}$	Scheme	ω_e/cm^{-1}	$\delta\omega_e/\text{cm}^{-1}$	Ref.
Na ₂	154.236	42	159.6069	5.3709	{NaK-K ₂ }			
K ₂	91.54	43	93.1481	1.6081	{KCs-Cs ₂ }	94.80	3.26	18
Rb ₂	60.1	44	59.5688	-0.5312	{RbCs-Cs ₂ }			
Cs ₂	42.6524	45	42.3544	-0.2980	{RbCs-Rb ₂ }	43.133	0.48	45
			43.2035	0.5511	{KCs-K ₂ }			
$b^3\Pi$								
NaK	120.41	46	118.9115	-1.4985	{K ₂ +Na ₂ }	121.71	1.30	18
			120.2066	-0.2034	{Na ₂ +KCs-Cs ₂ }	120.06	-0.35	59
KCs	68.4	47	67.6263	-0.7737	{K ₂ +RbCs-Rb ₂ }	71.55	3.15	52
			67.9001	-0.4999	{K ₂ +Cs ₂ }			
			68.4780	0.0780	{Cs ₂ +NaK-Na ₂ }	68.84	0.44	55
RbCs	50.883	48	51.4494	0.5664	{Rb ₂ +KCs-K ₂ }	53.05	2.17	56
			51.0835	0.2005	{Rb ₂ +Cs ₂ }			
$A^1\Sigma_u^+$								
Li ₂	255.4771	60	260.2155	4.7384	{LiNa-Na ₂ }			
Na ₂	117.3881	42	118.8815	1.4934	{LiNa-Li ₂ }			
$A^1\Sigma^+$								
LiNa	188.0328	61	186.6403	-1.3925	{Li ₂ +Na ₂ }			
LiK	137.0821	66	139.3691	2.2870	{Li ₂ +KCs-Cs ₂ [#] }			
NaRb	65.7	67	67.8023	2.1023	{Na ₂ +RbCs-Cs ₂ [#] }	63.51	-2.19	67
						77.1	11.4	67
KCs	49.8	47	49.2666	-0.5333	{Cs ₂ [#] +LiK-Li ₂ }	50.30	0.50	52
						48.30	-1.5	55
RbCs	34.98	48	34.1441	-0.8359	{Cs ₂ [#] +NaRb-Na ₂ }			

[#] ω_e (33.0055 cm⁻¹) from Ref. 45.

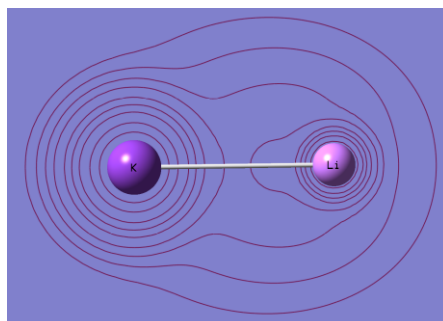
Figure S1



(a) Li₂



(b) LiNa



(c) LiK

Figure S1. Total electronic densities in the ground states of (a). Li₂; (b). LiNa; and (c). LiK molecules. The data are calculated using the *Gaussian 03* package⁷³ at Hartree-Fock/6-311++g(3df,3dp) level. Parameters are the same for different molecules. Resolution=0.1 Å and full density matrixes are used.

The information on the distribution of electronic densities in the ground states of Li₂, LiNa, and LiK presented in Figure S1 show that the total electronic density around the Li atom in Li₂ is more close to that in LiNa than in LiK. Comparing with the data in Figure 3 in the text, it is clear that the similarity in chemical environment of related atoms in the relevant molecules is important for the two-molecule schemes to produce reliable results.

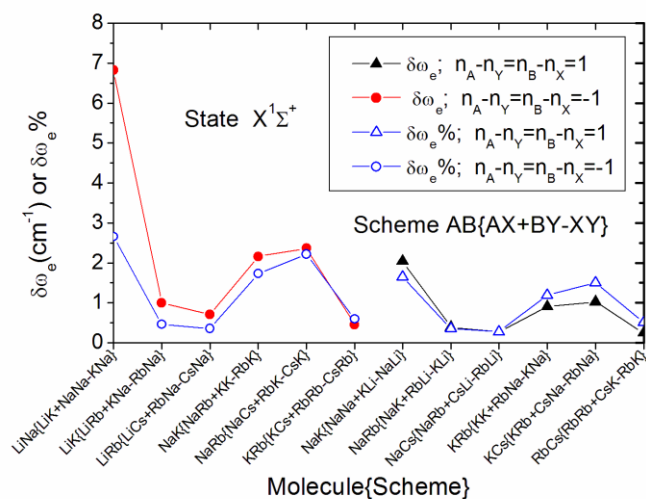


Figure S2 Errors from the AB{AX+BY-XY} schemes with $(n_B-n_X) \times (n_A-n_Y) = -1$. All the errors are less than zero in this figure.

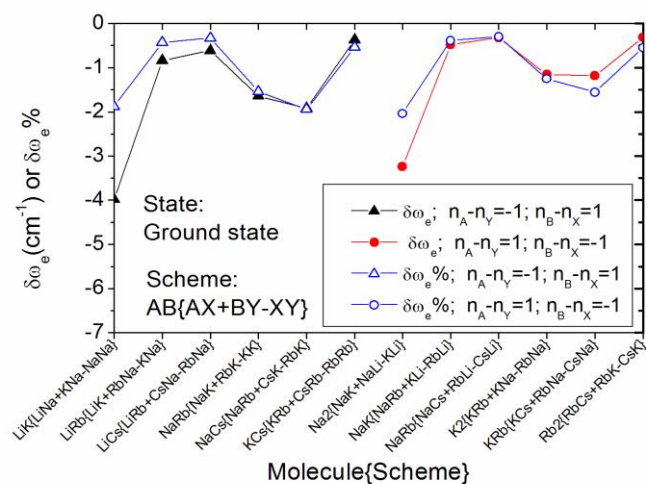


Figure S3 Errors from the AB{AX+BY-XY} schemes with $(n_B-n_X) \times (n_A-n_Y) = 1$. All the errors are greater than zero in this figure.

From Figures S2-S3 it is clear that the sign of the error from the AB{AX+BY-XY} schemes is the same as the sign of $(n_B-n_X) \times (n_A-n_Y)$.

Table S3 Harmonic frequencies from the AB{AX+BY-XY} and the AB{A₂+BC-C₂} schemes for some sets of the ground-state molecules.*

	$\omega_{e,obs./cm^{-1}}$	Refs	$\omega_{e,calc./cm^{-1}}$	$\omega_{e,calc.}-\omega_{e,obs./cm^{-1}}$	$\delta\omega_e\%^\#$	Scheme/molecule set
						{LiO,NaO,NaCl,LiCl}
NaCl	364.6842	23	364.5714	-0.1128	-0.0309	{NaO+LiCl-LiO}
LiO	814.64	23	814.1981	-0.4419	-0.0542	{LiCl+NaO-NaCl}
LiCl	642.95453	23	643.2152	0.2607	0.0405	{LiO+NaCl-NaO}
NaO	492.3	23	492.4889	0.1889	0.0384	{LiO+NaCl-LiCl}
						{AlO,BiO,BiS,AlS}
BiO	692.4	24	692.7788	0.3788	0.0547	{AlO+BiS-AlS}
AlO	979.4852	23	978.7619	-0.7233	-0.0738	{BiO+AlS-BiS}
AlS	617.1169	23	617.3810	0.2641	0.0428	{AlO+BiS-BiO}
BiS	408.71	24	408.5648	-0.1452	-0.0355	{AlS+BiO-AlO}
						{BH,SiH,BF,SiF}
BH	2366.7296	23	2366.9387	0.2091	0.0088	{SiH+BF-SiF}
SiH	2042.5229	23	2042.3813	-0.1416	-0.0069	{BH+SiF-BF}
BF	1402.1587	23	1401.8306	-0.3281	-0.0234	{BH+SiF-SiH}
SiF	837.32507	23	837.4386	0.1135	0.0136	{BF+SiH-BH}
						{GaO,AlO,AlH,GaH}
AlO	979.4852	23	980.0529	0.5677	0.0580	{GaO+AlH-GaH}
GaH	1605.0	17	1605.3793	0.3793	0.0236	{AlH+GaO-AlO}
AlH	1682.3747	23	1682.0967	-0.2780	-0.0165	{GaH+AlO-GaO}
GaO	767.5	24	767.1474	-0.3526	-0.0459	{AlO+GaH-AlH}
						{HF,CuF,CuO,OH}
CuF	622.65	24	622.4949	-0.1551	-0.0249	{HF+CuO-OH}
OH	3737.761	23	3735.5828	-2.1782	-0.0583	{HF+CuO-CuF}
HF	4138.4	23	4141.3901	2.9901	0.0723	{OH+CuF-CuO}
CuO	640.17	24	640.3174	0.1474	0.0230	{OH+CuF-HF}
						{KF,CsF,KBr,CsBr}
CsBr	149.66	24	149.6699	0.0099	0.0066	{KBr+CsF-KF}
KBr	213.0	24	212.9850	-0.0150	-0.0070	{KF+CsBr-CsF}
CsF	352.56	24	352.5167	-0.0433	-0.0123	{KF+CsBr-KBr}
KF	428.0	24	428.0595	0.0595	0.0139	{CsF+KBr-CsBr}
						{BrNa+RbCl-NaCl}
RbBr	169.46	24	169.593	0.13	0.08	{ClNa+RbBr-NaBr}
RbCl	228	24	227.8043	-0.20	-0.09	{NaCl+BrRb-ClRb}
NaBr	302.1	24	301.7728	-0.33	-0.11	{NaBr+ClRb-BrRb}
NaCl	364.6842	23	365.1342	0.45	0.12	{BaBr,SrBr,BaI,SrI}
						{SrBr+BaI-SrI}
BaBr	193.8	24	193.8626	0.0626	0.0323	{BaBr+SrI-BaI}
SrBr	216.5	24	216.4277	-0.0723	-0.0334	{SrBr+BaI-BaBr}
SrI	174.1	24	174.1470	0.0470	0.0270	{SrI+BaBr-SrBr}
BaI	152.30	24	152.2600	-0.0400	-0.0263	{SrI+BaBr-SrBr}
						{HI,HAu,Au ₂ ,AuI}

HAu	2305.5008	70	2303.7743	-1.7265	-0.0749	{HI+Au ₂ -AuI}
HI	2309.0	24	2310.7335	1.7335	0.0751	{HAu+AuI-Au ₂ }
AuI	215.77	74	215.6610	-0.1090	-0.0505	{HI+Au ₂ -HAu}
Au ₂	190.9	10	190.9964	0.0964	0.0505	{AuI+AuH-HI}
						AB{A ₂ +BC-C ₂ }
NH	3282.72	23	3282.6816	-0.0384	-0.0012	{N ₂ +PtH-Pt ₂ }
PtH	2294.68	24	2294.6940	0.0140	0.0006	{Pt ₂ +NH-N ₂ }
CuBr	314.8	24	314.7690	-0.0310	-0.0098	{Br ₂ +CuI-I ₂ }
CuI	264.5	24	264.5221	0.0221	0.0084	{I ₂ +CuBr-Br ₂ }
BO	1885.286	23	1884.0912	-1.1948	-0.0634	{B ₂ +ZrO-Zr ₂ }
OZr	969.7	24	968.9790	-0.7210	-0.0743	{Zr ₂ +BO-B ₂ }
VO	1011.0	24	1010.2841	-0.7159	-0.0708	{V ₂ +VO-W ₂ }
WO	1059.9	24	1060.9334	1.0334	0.0975	{W ₂ +VO-V ₂ }
BiSb	220.0	24	219.9625	-0.0375	-0.0171	{Sb ₂ +BiF-F ₂ }
BiF	511.0	17	511.1070	0.1070	0.0209	{F ₂ +BiSb-Sb ₂ }

* The experimental harmonic frequencies of the homonuclear molecules used in the AB{A₂+BC-C₂}

schemes are taken from refs.23 and 10, otherwise 24.

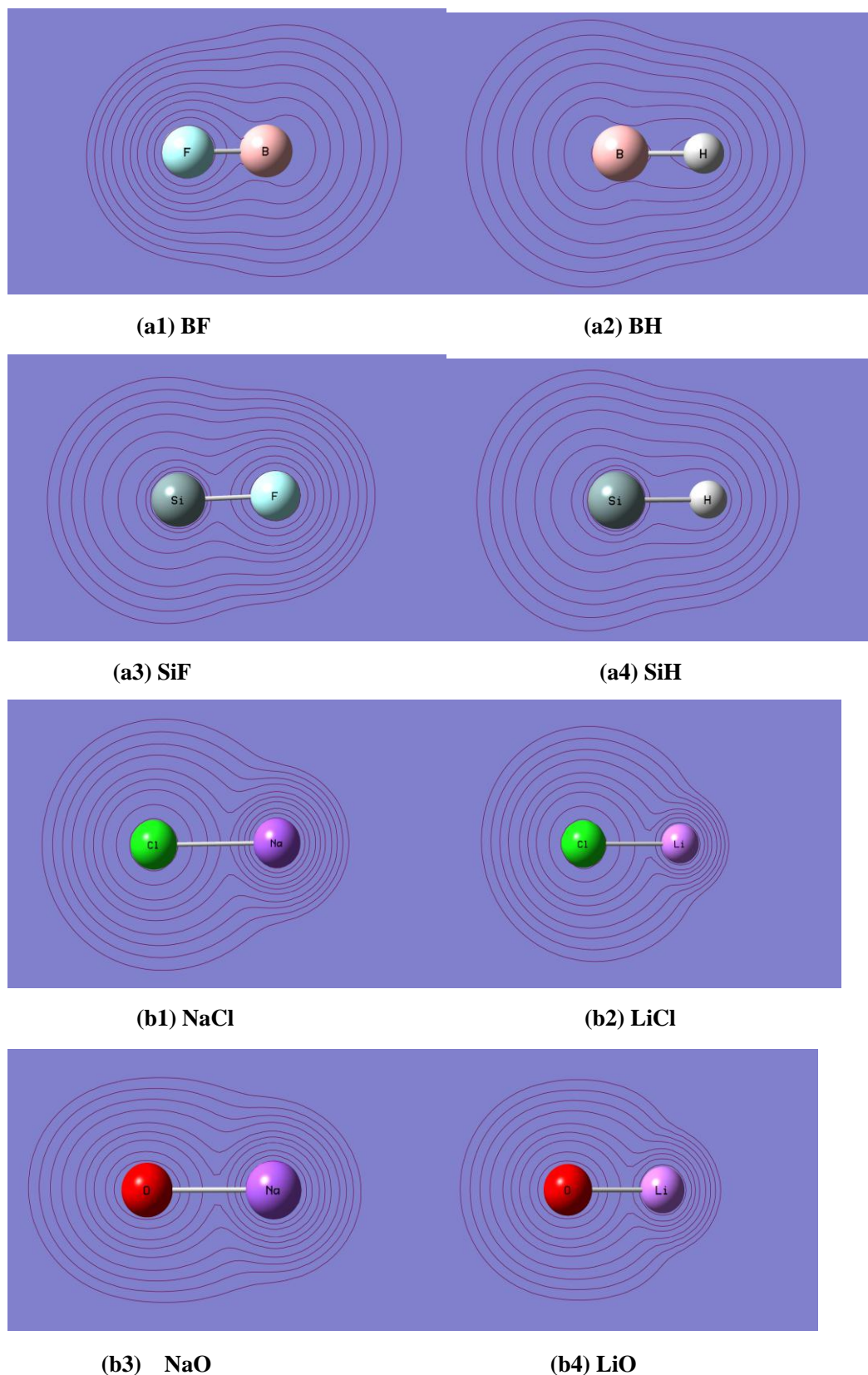


Figure S4 Total electronic densities in the ground states of molecules in (a) {BH, SiH, BF, SiF} and (b) {LiO, LiCl, NaO, NaCl} sets: (a1) BF; (a2) BH; (a3) SiF; (a4) SiH; (b1) NaCl; (b2) LiCl; (b3) NaO; (b4) LiO. The data are calculated using the *Gaussian 03* package⁷³ at the B3LYP/6-311++g(3df,3dp) level. Resolution=0.1 Å. Parameters are the same for different molecules. Full density matrixes are used.

Section S1 Results for molecules from groups IIA & VIA

Different schemes are tested for molecules such as BeO, BeS, MgO, MgS, CaO, CaS, SrO, SrS, BaO, and BaS. For MgO, the {Mg₂+O₂}, {Mg₂+CaO-Ca₂}, {MgS+O₂-S₂}, {MgS+BeO-BeS}, and the {MgS+CaO-CaS} schemes are compared. The corresponding schemes and results for all these molecules are presented in Table S4. For the ground state of MgO, the errors of the ω_e show that the {MgS+CaO-CaS} scheme can provide acceptable data ($\delta\omega_e\%=2.5\%$). While the schemes involve van de Waals molecules such as Mg₂ and Ca₂ give results with larger errors ($\sim 90\%$). According to classical mechanics, all the schemes should produce the same results. The different results from different schemes demonstrate that quantum effects produce different force constants for the same atom in different molecules. As an atom in a van de Waals molecule, the force constant of Mg in Mg₂ is very small, and is far less than k_{Mg} in MgO. That is why the {Mg₂+O₂} scheme produces a result far less than the experimental data. The results of the {MgS+CaO-CaS} scheme provide supporting that the k_{Mg} in MgO and MgS are nearly the same, and the k_{O} in MgO and CaO are similar to each other. Similar reasons can be adopted to explain results from other schemes. This result indicates that the spring constant for an atom is related with the chemical bond of the molecule. For a given atom, to obtain a better prediction of the ω_e to other molecules, the chemical bond in one molecule should be similar to the one in the other molecule to be predicted.

For a given scheme, such as the AB{AX+BY-XY} scheme, there are some sets of molecules, such as {BaO, SrO, BaS, SrS}, in which the harmonic frequency of one molecule can be obtained from those of the other three molecules. The errors for the molecules in the same set are similar to each other. For example, in the {MgO,²³ MgS,²³ CaO,²⁴ CaS²⁴} set, the relative errors MgO, CaO, MgS and CaS are 2.5%, -2.4%, -1.5%, and 1.6%, respectively. In the {BaO,²⁴ SrO,⁶² BaS,⁶⁴ SrS⁶³} set, the relative errors SrO, BaO, SrS and BaS are 0.68%, -0.74%, -0.41%, and 0.44%, respectively.

Table S4 Harmonic frequencies obtained from theory of atomic spring constants for the $X^1\Sigma^+$ states of BeO, BeS, MgO, MgS, CaO, CaS, SrO, SrS, BaO, and BaS.

Molecule {Scheme}	$\omega_{e,obs.}/\text{cm}^{-1}$	Ref.	$\omega_{e,calc.}/\text{cm}^{-1}$	$\omega_{e,calc.}-\omega_{e,obs.}/\text{cm}^{-1}$	$\delta\omega_e\%^\#$
BeO {BeS+SO-S ₂ }	1487.3200	23	1352.2236	-135.0964	-9.08%
BeS {BeO+S ₂ -SO}	997.9400	23	1060.9146	62.9746	6.31%
{BeO,BeS,MgO,MgS} set:					
BeO {BeS+MgO-MgS}	1487.32	23	1847.3310	360.0110	24.21%
BeS {BeO+MgS-MgO}	997.94	23	913.5988	-84.3412	-8.45%
MgO {BeO+MgS-BeS}	785.2183	23	728.0463	-57.1720	-7.28%
MgS {MgO+BeS-BeO}	528.74	23	559.1131	30.3731	5.74%
{MgO,MgS,CaO,CaS} set:					
MgO {MgS+CaO-CaS}	785.2183	23	804.9457	19.7274	2.51%
CaO {MgO+CaS-MgS}	732.10	24	714.4225	-17.6775	-2.41%
MgS {MgO+CaS-CaO}	528.74	23	520.6415	-8.0985	-1.53%
CaS {MgS+CaO-MgO}	462.23	24	469.5787	7.3487	1.59%
{MgO,SrO,MgS,SrS} set:					
MgO {SrO+MgS-SrS}	785.2183	23	830.1899	44.9716	5.73%
SrO {MgO+SrS-MgS}	653.3083	62	622.0852	-31.2232	-4.78%
MgS {MgO+SrS-SrO}	528.7400	23	511.5692	-17.1708	-3.25%
SrS {MgS+SrO-MgO}	388.2643	63	401.0974	12.8331	3.31%
{CaO,BaO,CaS,BaS} set:					
CaO {BaO+CaS-BaS}	732.1000	24	760.5091	28.4091	3.88%
BaO {CaO+BaS-CaS}	669.7600	24	645.3766	-24.3834	-3.64%
CaS {BaS+CaO-BaO}	462.2300	24	452.0721	-10.1579	-2.20%
BaS {CaS+BaO-CaO}	379.3828	64	388.1644	8.7816	2.31%
{CaO,SrO,CaS,SrS} set:					
CaO {SrO+CaS-SrS}	732.1000	24	754.6920	22.5920	3.09%
SrO {CaO+SrS-CaS}	653.3083	62	635.8591	-17.4492	-2.67%
CaS {SrS+CaO-SrO}	462.2300	24	454.0063	-8.2237	-1.78%
SrS {CaS+SrO-CaO}	388.2643	63	395.0472	6.7829	1.75%
{SrO,BaO,SrS,BaS} set:					
SrO {BaO+SrS-BaS}	653.3083	62	657.7731	4.4647	0.68%
BaO {SrO+BaS-SrS}	669.7600	24	664.7731	-4.9869	-0.74%
SrS {BaS+SrO-BaO}	388.2643	63	386.6671	-1.5972	-0.41%
BaS {SrS+BaO-SrO}	379.3828	64	381.0536	1.6708	0.44%

$\# \delta\omega_e\% = 100\%(\omega_{e,calc.}-\omega_{e,obs.})/\omega_{e,obs.}$. The observed data are taken from Ref.23 for O₂, S₂, Mg₂, and Ref.24 for Ca₂.

Section S2 Results for group IB molecules

For the groups IB atoms, results from their diatomic molecules and their hydrides are compared in Figure S5. The results show that the Cu, Ag, Au, and H compounds can provide reliable force constants and ω_e from the present approach. Though H is not belong to group IB, and the mass of H is different much to those of the IB atoms, it can be used to produce better harmonic frequencies from its spring constant. The errors for CuH, AgH, and AuH from the AB{A₂+B₂} scheme are about 3%. Despite of the difference in the masses of H and Au, there are similar in the electronic configurations (one electron in the outmost shell) and the electronegativities. Their electronegativities are 2.4, 1.9, 1.9, and 2.1 for Au, Ag, Cu, and H respectively.⁸ The results for molecules from same groups also demonstrate that atoms with similar electronegativities produce accurate data easily from both the AB{A₂+B₂} and the AB{AX+BY-XY} schemes.

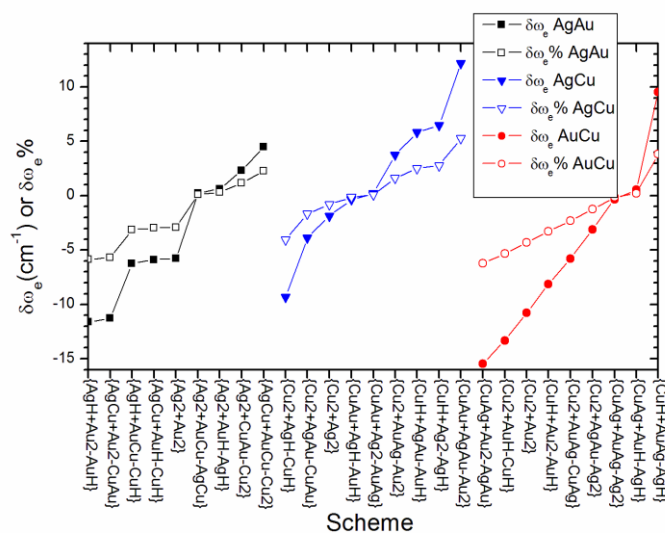


Figure S5 Errors for AuCu, AgCu, and AgAu from molecules of Group IB atoms and their hydrides. The experimental ω_e are from ref.68 for CuH, AuH, and AgH; ref.65 for AgAu; ref.24 for AuCu, AgCu; and ref.10 for Cu₂, Ag₂, and Au₂.

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