Supporting Information

Electronic Structure and Chemical bonding of the MoBe molecule

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Table S1. Equilibrium bond distances (R_e/Å), absolute energies (E/Hartree) and relative energy differences with respect to the ground state (T_e / *e*V , cm^{-1} and kcal/mol) for 43 calculated electronic states of MoBe at the SA-CASSCF/ aug-cc-pV5Z level of theory.

State	R_e	*E*		T_e	
$^3\Pi(1)$	**2.390**	**-81.858736**	**2.089**	**16849**	**48.17**
$^3\Delta(1)$	**2.096**	**-81.857463**	**2.124**	**17129**	**48.97**
$^3\Sigma^+(1)$	**2.409**	**-81.852850**	**2.249**	**18141**	**51.87**
$^3\Phi$	2.151	-81.849824	2.332	18805	53.77
$^3\Delta(2)$	2.226	-81.846580	2.420	19517	55.80
$^3\Pi(2)$	2.179	-81.844497	2.476	19974	57.11
$^3\Sigma^-$	2.136	-81.842142	2.541	20491	58.59
$^3\Pi(3)$	2.234	-81.839283	2.618	21119	60.38
$^3\Delta(3)$	2.330	-81.838602	2.637	21268	60.81
$^3\Gamma$	2.379	-81.827849	2.930	23628	67.56
$^3\Sigma^+(2)$	2.375	-81.827300	2.944	23749	67.90
$^5\Sigma^+(1)$	**2.474**	**-81.917524**	**0.489**	**39467**	**11.28**
$^5\Pi(1)$	**2.293**	**-81.894125**	**1.126**	**9082**	**25.97**
$^5\Pi(2)$	2.320	-81.874362	1.664	13420	38.37
$^5\Sigma^+(2)$	2.373	-81.872569	1.713	13813	39.49
$^5\Phi$	2.321	-81.866087	1.889	15236	43.56
$^5\Delta(1)$	2.419	-81.865747	1.898	15310	43.77
$^5\Sigma^+(3)$	2.485	-81.864684	1.927	15544	44.44
$^5\Delta(2)$	2.456	-81.860279	2.047	16510	47.21
$^5\Pi(3)$	2.671	-81.856334	2.154	17376	49.68
$^5\Gamma$	2.505	-81.851048	2.298	18537	53.00
$^5\Sigma^-$	2.401	-81.847590	2.392	19296	55.17
$^7\Sigma^+(1)$	**2.497**	**-81.935507**	**0.000**	**0**	**0.00**
$^7\Pi(1)$	**2.438**	**-81.877618**	**1.575**	**12705**	**36.33**
$^7\Sigma^+(2)$	2.521	-81.866841	1.868	15070	43.09
$^7\Sigma^+(3)$	2.746	-81.847444	2.396	19327	55.26
$^7\Pi(2)$	2.560	-81.840098	2.596	20940	59.87
$^7\Phi$	2.560	-81.834666	2.744	22132	63.28
$^7\Delta(1)$	2.735	-81.832735	2.797	22556	64.49
$^7\Pi(3)$	2.574	-81.830490	2.858	23049	65.90
$^7\Delta(2)$	2.600	-81.823730	3.042	24532	70.14
$^7\Sigma^-(1)$	2.603	-81.821117	3.113	25106	71.78
$^7\Sigma^-(2)$	2.395	-81.794649	3.833	30915	88.39
$^9\Pi(1)^a$	**2.556**	**-81.847261**	**2.401**	**19368**	**55.38**
$^9\Sigma^+(1)$	**2.597**	**-81.833096**	**2.787**	**22477**	**64.26**
$^9\Sigma^-(1)$	2.461	-81.786737	4.048	32651	93.35
$^9\Pi(2)$	2.889	-81.773541	4.407	35547	101.63
$^9\Phi$	2.875	-81.762959	4.695	37870	108.28
$^9\Delta(1)$	2.979	-81.762877	4.697	37888	108.33
$^9\Sigma^-(2)$	2.957	-81.760551	4.761	38398	109.79
$^9\Pi(3)$	2.903	-81.760527	4.761	38404	109.80
$^9\Delta(2)$	2.607	-81.750254	5.041	40658	116.25
$^9\Sigma^+(2)$	3.450	-81.740240	5.313	42856	122.53

Table S2. Bond distances (R_e/Å) and absolute energies (E_e/Hartree) of nine electronic state of MoBe at CASSCF, MRCISD, MRCISD+Q/aug-cc-pV5Z(-PP) levels of theory.

State	Method	R_e	E_e
	MRCISD	2.481	-82.072252
	MRCISD+Q	2.462	-82.080312
$^5\Sigma^+$	CASSCF	2.488	-81.925802
	MRCISD	2.400	-82.047564
	MRCISD+Q	2.392	-82.056436
$^5\Pi$	CASSCF	2.286	-81.907372
	MRCISD	2.181	-82.039743
	MRCISD+Q	2.177	-82.049643
$^7\Pi$	CASSCF	2.464	-81.888875
	MRCISD	2.365	-82.014596
	MRCISD+Q	2.359	-82.025087
$^3\Delta$	CASSCF	2.087	-81.858590
	MRCISD	2.045	-82.004734
	MRCISD+Q	2.047	-82.016213
$^3\Pi$	CASSCF	2.317	-81.861477
	MRCISD	2.264	-81.999311
	MRCISD+Q	2.266	-82.010347
$^3\Sigma^+$	CASSCF	2.404	-81.855214
	MRCISD	2.338	-81.992645
	MRCISD+Q	2.333	-82.004309
$^9\Pi$	CASSCF	2.661	-81.857551
	MRCISD	2.581	-81.966914
	MRCISD+Q	2.579	-81.974270
$^9\Sigma^+$	CASSCF	2.851	-81.854930
	MRCISD	2.752	-81.956397
	MRCISD+Q	2.787	-81.962155

Table S3. Population Analysis of the $X^7\Sigma^+$ state.

Method	Population Analysis	Atomic population distributions (Mo/Be)
MRCISD/cc-pVTZ(-PP)	Mulliken	$5s^{1.11}5p_z^{0.23}5p_x^{0.01}5p_y^{0.01}4d_{z^2}^{1.00}4d_{x^2-y^2}^{0.99}4d_{xz}^{0.94}4d_{yz}^{0.94}4d_{xy}^{0.99}$ /$2s^{1.24}2p_z^{0.31}2p_x^{0.08}2p_y^{0.08}$
MRCISD/aug-cc-pV5Z(-PP)	Mulliken	$5s^{0.96}5p_z^{0.13}5p_x^{0.01}5p_y^{0.01}4d_{z^2}^{0.99}$ $4d_{xz}^{0.95}4d_{yz}^{0.95}4d_{x^2-y^2}^{0.99}$ $4d_{xy}^{0.99}$ / $2s^{1.47}2p_z^{0.33}2p_x^{0.08}2p_y^{0.08}$
MRCISD/aug-cc-pV5Z(-PP)	NPA	$5s^{1.06}5p_z^{0.07}5p_x^{0.01}5p_y^{0.01}4d_{z^2}^{0.95}4d_{x^2-y^2}^{1.00}4d_{xz}^{0.98}4d_{yz}^{0.98}4d_{xy}^{1.00}$ /$2s^{1.60}2p_z^{0.20}2p_x^{0.03}2p_y^{0.03}$

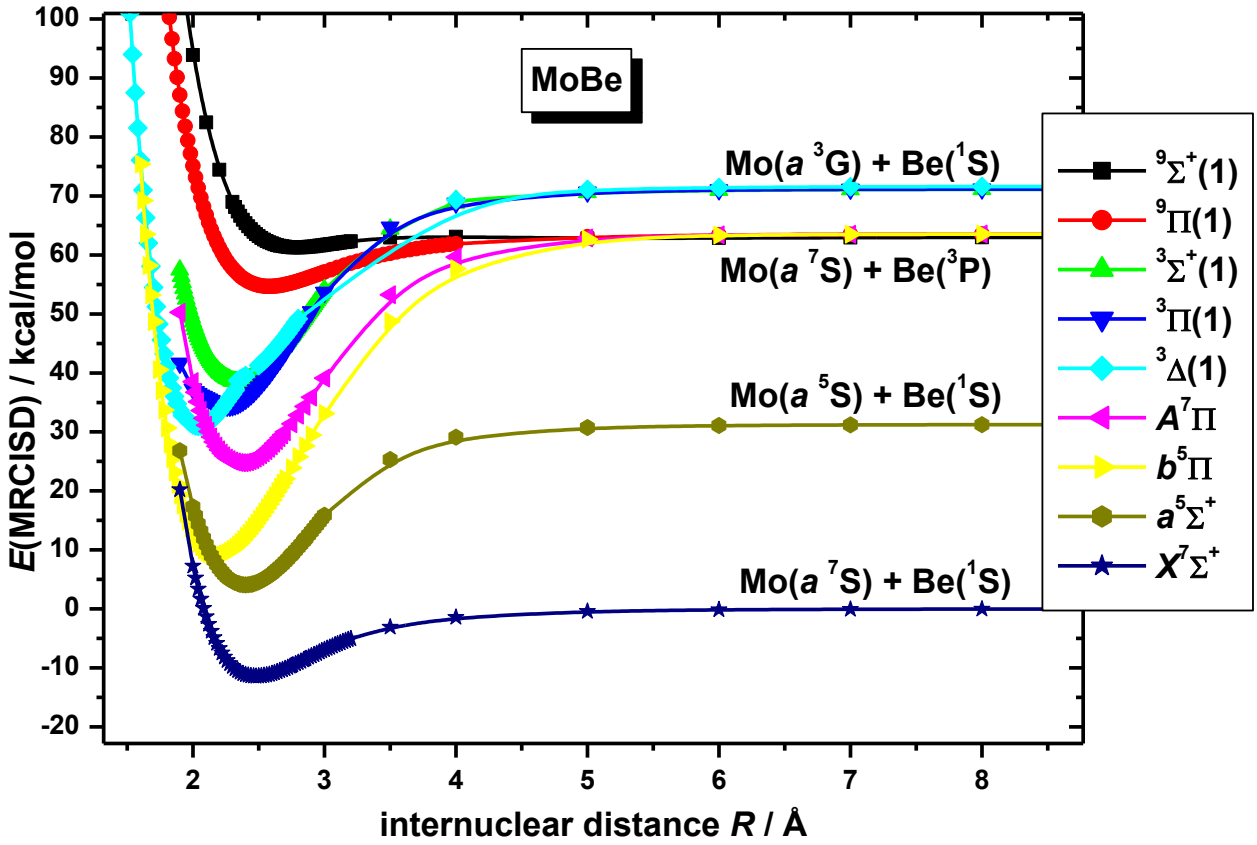

Figure S1. PECs of the selected states of MoBe at the MRCISD/aug-cc-pV5Z(-PP) computational level. The Mo($a\,^7$S) + Be($\,^1$S) limit, to which the $X\,^7\Sigma^+$ state correlates, is used to define the zero of energy.