Supporting information

Valence Electron and Chemical State Analysis of $Be_{12}M$ (M = Ti, V) Beryllides by Soft X-ray Emission Spectroscopy

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Table S1 Lattice parameters of Be, $Be_{12}Ti$, $Be_{12}V$, and BeO obtained by the structural optimization in the DFT calculations compared with the experimental ones.[1–4] The calculated lattice parameters agreed well with the experimental ones.

	Calculation		Experimental	
	a (Å)	*c* (Å	*a* (Å)	*c* (Å)
Be	2.257	3.587	2.287[a]	3.583[a]
$Be_{12}Ti$	7.430	4.235	7.35[b]	4.19[b]
$Be_{12}V$	7.215	4.147	7.278[c]	4.212[c]
BeO	2.705	4.395	2.698[d]	4.378[d]

a Reference 1

b Reference 2

c Reference 3

d Reference 4

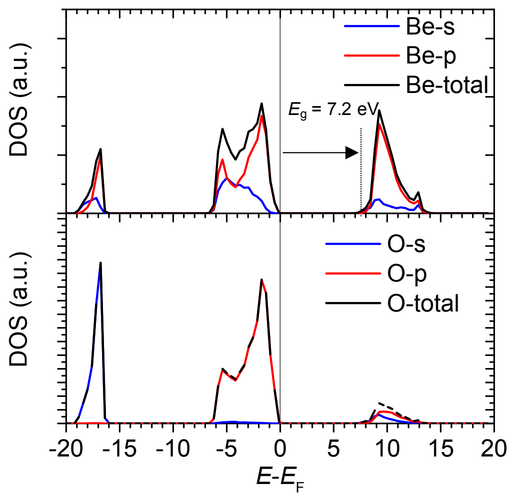

Fig. S1 Partial density of states (DOSs) of BeO plotted with the energy referenced to Fermi energy E_F. Black, blue, red, and green solid lines represent DOSs of total, *s*, and *p* states. The band gap energy of BeO was estimated to be 7.2 eV, which were comparable with the previous calculated values of 7.0 and 7.54 eV.[5,6] The calculated band gap was underestimated from the experimental band gap of BeO (10.6 eV).[7] The partial DOS Be-2*p* convoluted with the Gaussian function is compared with the experimental Be-Kα spectrum from the BeO specimen in Fig. 6.

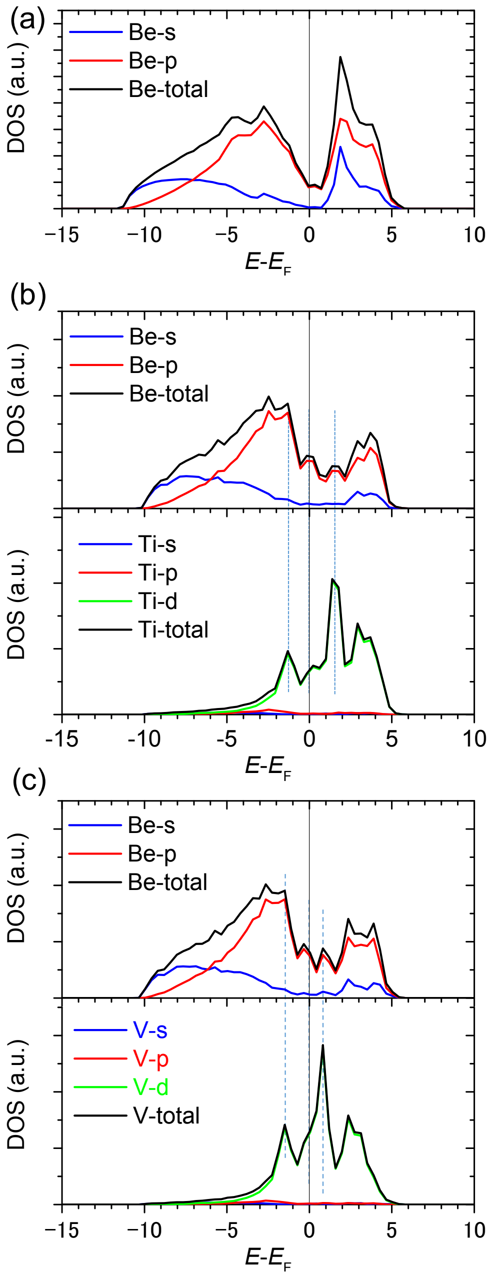

Fig. S2 Density of states in metallic Be (a), $Be_{12}Ti$ (b), and $Be_{12}V$ (c) with the energy referenced to the Fermi levels E_f. Black, blue, red, and green solid lines represent total, *s*, *p*, and *d* states. The DOSs of Be with the energy referenced with the Be-1*s* centroid are shown in Fig. 3. The valence electron structure of Be in $Be_{12}Ti$ and $Be_{12}V$ were altered from that of Be in metallic Be. The hybridized peaks of O 2*p* and Ti/V 3*d* states shown by blue dashed lines near the Fermi levels ($E - E_F = 0$) were seen in $Be_{12}Ti$ and $Be_{12}V$.

References

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