Supplementary Information (SI) for Journal of Materials Chemistry C. This journal is © The Royal Society of Chemistry 2025



Fig. S1 Structures of Ho³⁺, Yb³⁺-codoped Bi₂WO₆ with Bi³⁺ substitution **Table S1** Static energies of the optimized structures of Ho³⁺. Yb³⁺-codoped Bi₂WO₆

I able SI		gies of the	optimized st	fuctures of filo	, 10	$=$ coupped $B1_2 \le 0$	6
Structure number	(1)	(2)	(3)	(4)	(5)	(6)	(7)
Static energy (eV)	534.27	534.11	534.19	534.08	534.12	534.18	534.17
			a = 12 1 1		1 21		

Fig. S1 shows the possible structures of Bi^{3+} lattice sites in Ho^{3+} , Yb^{3+} -codoped Bi_2WO_6 , which are irreducible structures after accounting for the crystal symmetry and periodicity characteristics. Table S1 shows the static energies of the structures obtained after structural optimization (atom positions only) via VASP.



Fig. S2 Structures of K⁺, Ho³⁺, and Yb³⁺-codoped Bi₂WO₆ with Bi³⁺ substitution **Table S2** Static energies of the K⁺, Ho³⁺, and Yb³⁺-codoped Bi₂WO₆ structures after optimization

	8	,)	4	. 0		
Structure number	(1)	(2)	(3)	(4)	(5)	(6)	(7)
Static energy (eV)	529.01	529.32	528.85	528.96	529.08	529.03	529.19
Structure number	(8)	(9)	(10)	(11)	(12)	(13)	(14)
Static energy (eV)	529.09	529.16	528.89	528.96	529.25	529.04	529.01

Structure number	(15)	(16)	(17)	(18)	(19)	(20)	(21)
Static energy (eV)	528.60	528.90	529.10	528.76	529.15	528.72	529.12
Structure number	(22)	(23)	(24)	(25)	(26)	(27)	(28)
Static energy (eV)	529.14	528.97	529.21	529.05	528.90	529.12	528.64
Structure number	(29)	(30)	(31)	(32)	(33)	(34)	(35)
Static energy (eV)	529.04	529.27	528.77	529.07	528.97	528.85	528.80
Structure number	(36)	(37)	(38)	(39)	(40)	(41)	(42)
Static energy (eV)	529.38	529.24	529.02	529.36	529.12	529.25	529.14

Fig. S2 shows the possible structures of the Bi³⁺ lattice sites in K⁺, Ho³⁺, and Yb³⁺-codoped Bi₂WO₆, which are irreducible structures after accounting for the crystal symmetry and periodicity characteristics. Table S2 shows the static energies of the structures obtained after structural optimization (atom positions only) via VASP.