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Evidence of an interlayer charge transfer route in $BiCu_{1-x}SeO$

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Supplementary Materials

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Figure.S1 Comparison of experimental XANES spectra of BiCuSeO and $BiCu_{1-x}SeO$ (x=0.015) at the Bi L_3-edge, Cu and Se *K*-edges.

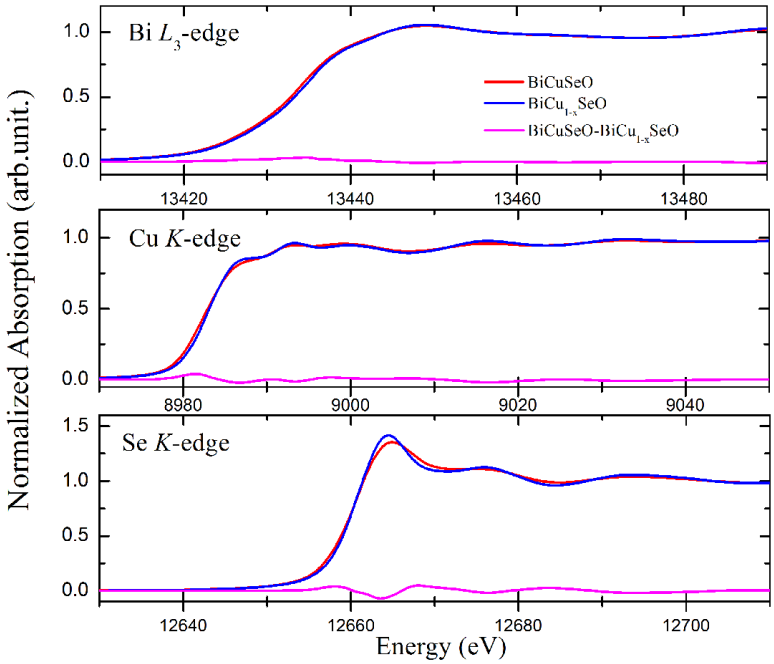

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Figure.S2 Comparison of spectra at Cu and Se *K*-edge among structural models with induced vacancies: 1) original structure; 2) one Cu vacancy near the excited atoms; 3) two Cu vacancies near the excited atoms in the trans and (4) cis geometry.

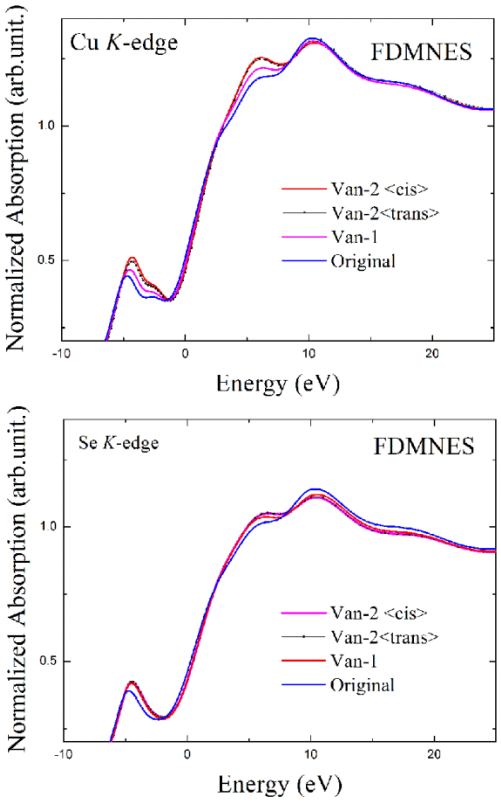

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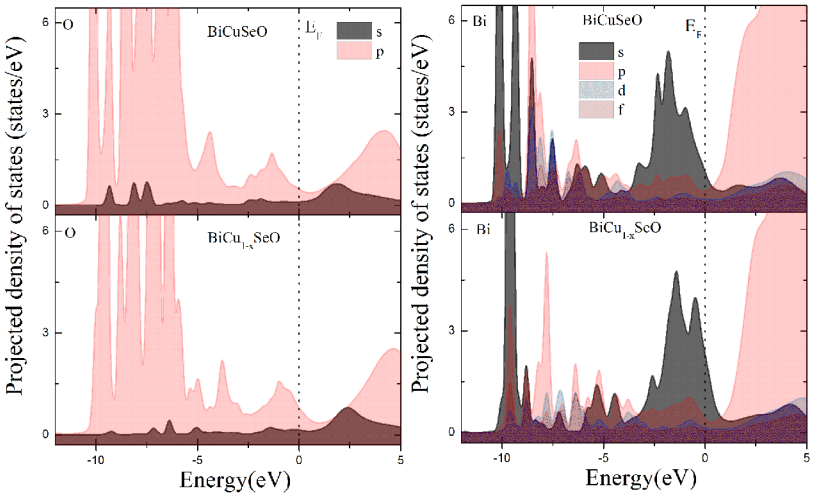
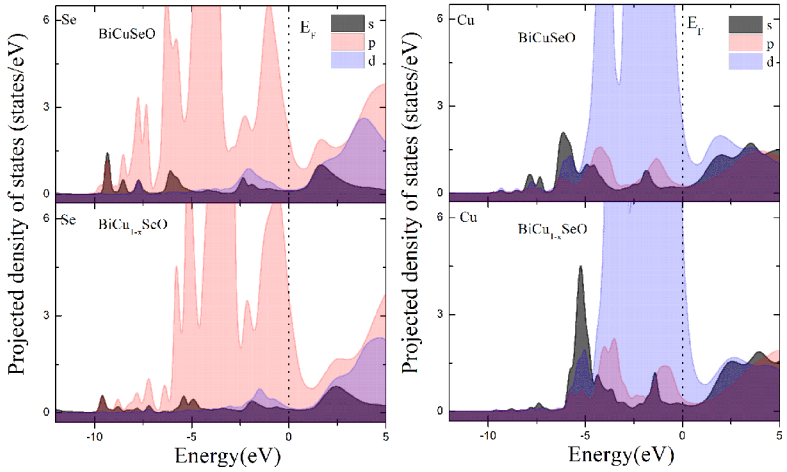
Figure.S3 Comparison among orbital-specific projected density of states between BiCuSeO (upper panels) and $BiCu_{1-x}SeO$ (x=0.015) (lower panels) of Cu *K*-edge XANES simulations: (panel a) O and Bi in the BiO layer and (panel b) Cu and Se in the CuSe layer.



(a)



(b)

Figure.S4 Comparison of total density of states for BiCuSeO, $BiCu_{1-x}SeO$, and $Bi_{1-x}SrCuSeO$, with x=0.0625

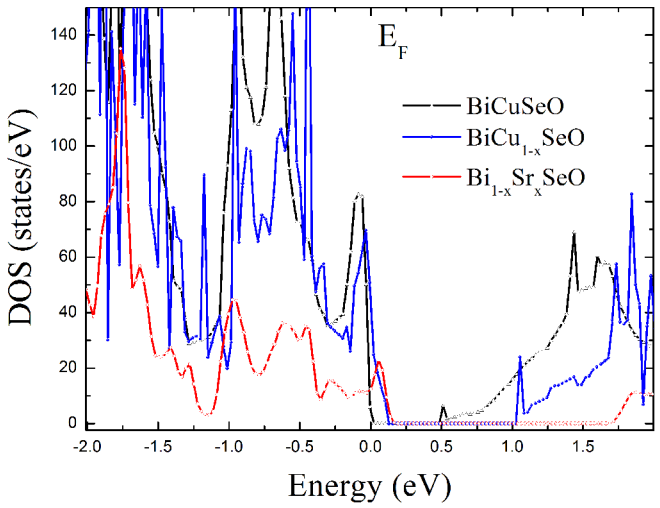


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Table S1. Electronic configurations and charge transfer parameters of BiCuSeO and $BiCu_{1-x}SeO$ (x=0.015) as from simulation of Cu and Se *K*-edges.

[a]CT stands for charge transfer; [b]Δ_{CT} refers to the charge transfer difference between BiCuSeO and $BiCu_{1-x}SeO$; Cu^0 and Se^0 are the excited Cu and Se absorber atoms, respectively.

(a) Cu *K*-edge

Atom	BiCuSeO				$BiCu_{1-x}SeO$				
	s	*p*	*d*	[a]CT	*s*	*p*	*d*	CT	[b]Δ_{CT}
Cu^0	1.036	1.225	10.237	-0.496	1.036	1.229	10.234	-0.498	0.002
Bi	1.920	1.886	10.519	0.676	1.922	1.869	10.517	0.693	-0.017
Se	1.942	3.992	0.339	-0.274	1.947	4.044	0.307	-0.298	0.024
Cu	0.650	0.724	9.669	-0.042	0.650	0.723	9.667	-0.039	-0.003
O	1.902	4.396	0.058	-0.357	1.899	4.396	0.057	-0.353	-0.004

(b) Se *K*-edge

Atom	BiCuSeO				$BiCu_{1-x}SeO$				
	s	*p*	*d*	CT	*s*	*p*	*d*	CT	Δ_{CT}
Se^0	2.011	4.637	0.330	0.022	2.005	4.691	0.294	0.010	0.012
Bi	1.922	1.893	10.519	0.667	1.924	1.873	10.517	0.687	-0.020
Se	1.933	4.003	0.335	-0.272	1.939	4.055	0.305	-0.300	0.028
Cu	0.643	0.707	9.679	-0.029	0.643	0.705	9.677	-0.026	-0.003
O	1.903	4.406	0.058	-0.368	1.900	4.406	0.057	-0.363	-0.005

Table S2. Electronic configurations and charge transfer parameters of BiCuSeO and $Bi_{1-x}Sr_xCuSeO$ (x=0.015) as from simulation of Cu and Se *K*-edges. [a]CT stands for charge transfer; [b]Δ_{CT} refers to the charge transfer difference between BiCuSeO and $BiCu_{1-x}SeO$; Cu^0 and Se^0 are the excited Cu and Se absorber atoms, respectively.

Atom	(a) Cu *K*-edge								
	BiCuSeO				$Bi_{1-x}Sr_xCuSeO$				
	s	*p*	*d*	[a]CT	*s*	*p*	*d*	CT	[b]Δ_{CT}
Cu^0	1.036	1.225	10.237	-0.496	1.018	1.205	10.228	-0.450	-0.046
Bi	1.920	1.886	10.519	0.676	1.918	1.838	10.511	0.733	-0.057
Se	1.942	3.992	0.339	-0.274	1.932	4.000	0.324	-0.257	-0.017
Cu	0.650	0.724	9.669	-0.042	0.637	0.712	9.652	-0.002	-0.04
O	1.902	4.396	0.058	-0.357	1.895	4.519	0.057	-0.471	0.114
Sr	x	x	x	x	0.365	6.459	1.297	-0.120	-0.120
Atom	(b) Se *K*-edge								
	BiCuSeO				$Bi_{1-x}Sr_xCuSeO$				
	s	*p*	*d*	CT	*s*	*p*	*d*	CT	Δ_{CT}
Se^0	2.011	4.637	0.330	0.022	2.003	4.633	0.318	0.046	-0.024
Bi	1.922	1.893	10.519	0.667	1.920	1.845	10.511	0.724	-0.057
Se	1.933	4.003	0.335	-0.272	1.921	4.012	0.320	-0.254	-0.018
Cu	0.643	0.707	9.679	-0.029	0.632	0.696	9.661	.011	-0.04
O	1.903	4.406	0.058	-0.368	1.896	4.529	0.057	-0.482	0.114
Sr	x	x	x	x	0.365	6.460	1.295	-0.121	-0.121