Supporting information

Physical Chemistry Chemical Physics

Self-Emitting Blue and Red EuOX (X = F, Cl, Br, I) Materials: Band Structure, Charge Transfer Energy, and Emission Energy

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Table S1. Refinement Atomic Position for EuOX (X = F, Cl, Br, I) materials

EuOF					
Atom	**Site**	***x***	***y***	***z***	B_{iso}
Eu	6*c*	0	0	0.2418(1)	0.22(3)
O	6*c*	0	0	0.1219(5)	0.5(3)
F	6*c*	0	0	0.3702(4)	0.5(2)
EuOCl					
Atom	**Site**	***x***	***y***	***z***	B_{iso}
Eu	2*c*	0.25	0.25	0.1724(1)	0.09(4)
O	2*a*	0.75	0.25	0	0.5(3)
Cl	2*c*	0.25	0.25	0.6263(5)	0.4(1)
EuOBr					
Atom	**Site**	***x***	***y***	***z***	B_{iso}
Eu	2*c*	0.25	0.25	0.1447(1)	0.45(3)
O	2*a*	0.75	0.25	0	1.9(4)
Br	2*c*	0.25	0.25	0.6575(2)	0.77(5)
EuOI					
Atom	**Site**	***x***	***y***	***z***	B_{iso}
Eu	2*c*	0.25	0.25	0.1229(1)	0.53(4)
O	2*a*	0.75	0.25	0	0.4(3)
I	2*c*	0.25	0.25	0.6736(1)	0.546(2)

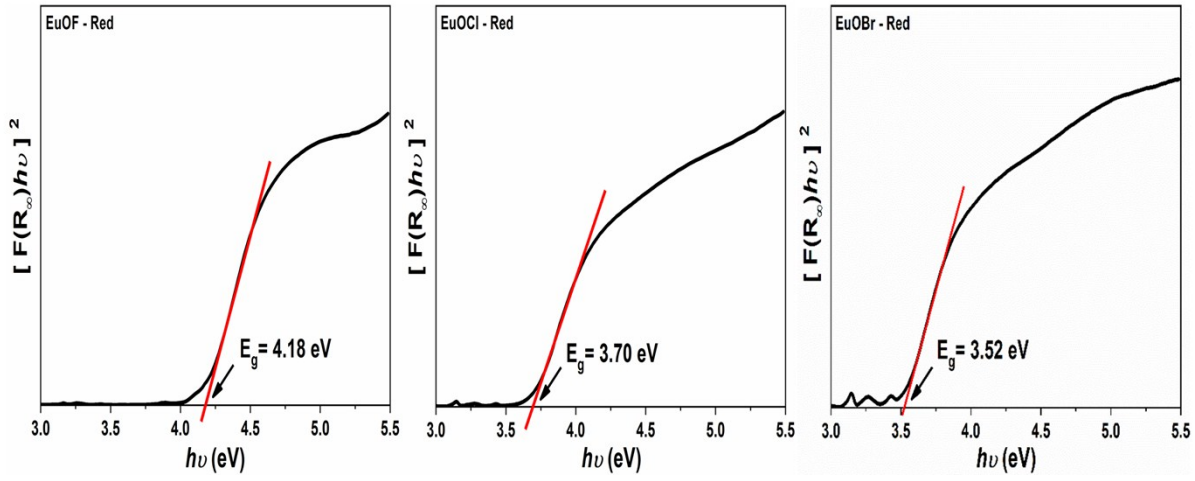

Figure S1. Band-gap energy (E_g) of EuOX (X = F, Cl, Br) materials using the Kubellka-Munk function.