Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Structural Analysis of Metal-doped Calcium Oxalate

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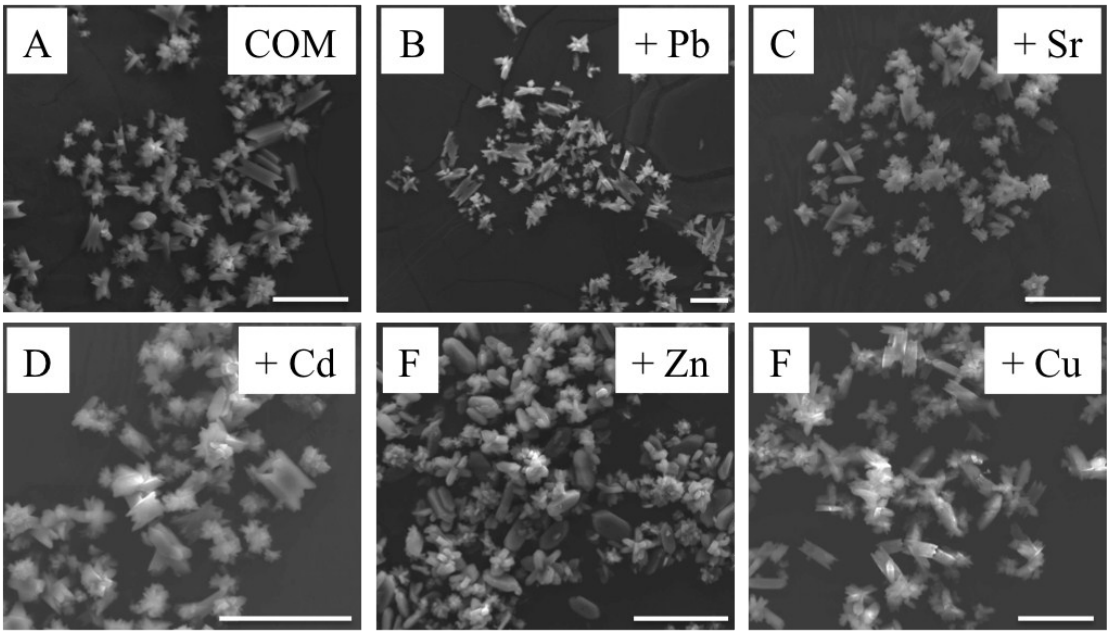

Figure S1. Overview of COM crystals grown in the absence (A) and in the presence of metal-containing solution (B−F). COM crystals appear as twin or as polycrystalline aggregates in all samples. However, the abundance of metals leads to distortion of crystal shape, as seen in Figure 1 in the example of a twinned crystal. Scale bars, 25 μm.

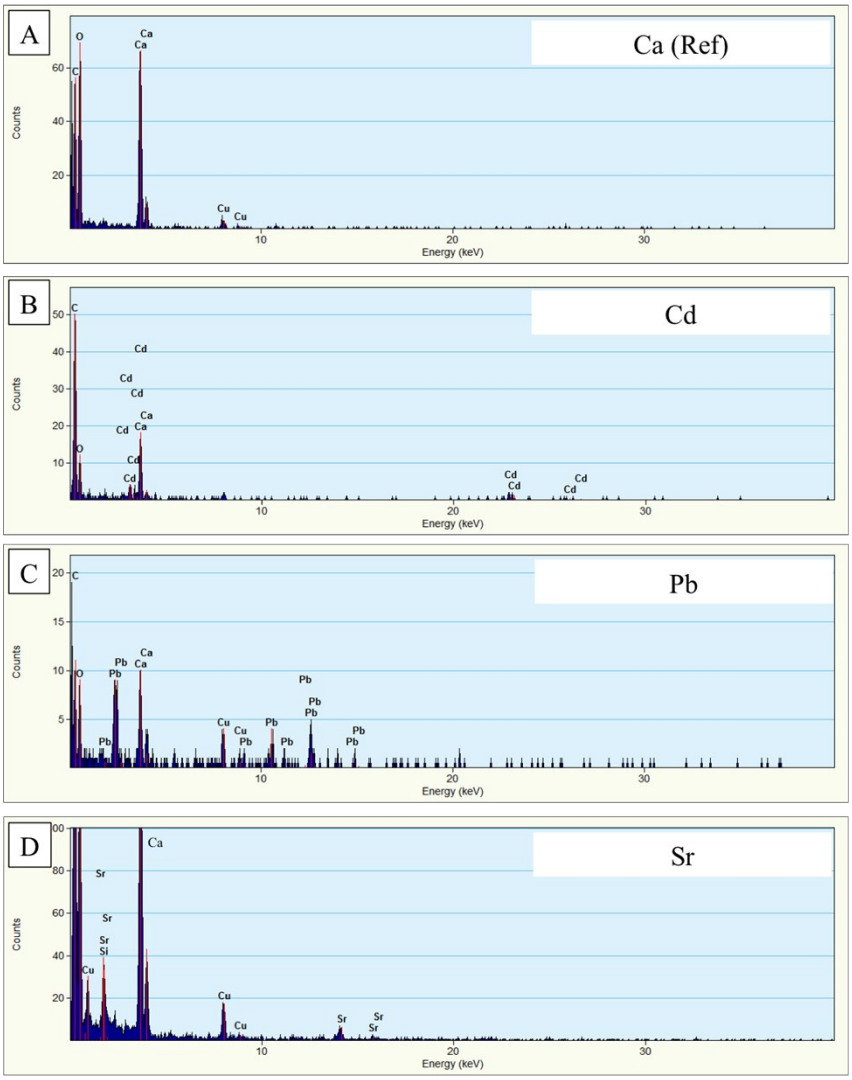

Figure S2. EDS analysis by TEM of the baseline COM reference (A) and metal-doped COM samples (B−D). The presence of elements in all metal-doped COM crystals is confirmed (B−D). Copper signals in EDS spectra remain from the TEM grids (A,C,D).

Table S1: Lattice constants of metal-doped COM as determined by the Rietveld refinement method.

	a	*b*	*c*	R_{wp}	GOF
COM	6.287(2)	14.558(1)	10.093(5)	7.81%	2.47
COM-Cd	6.283(4)	14.549(2)	10.09(1)	9.23%	2.54
COM-Cu	6.288(1)	14.5594(9)	10.090(5)	10.28%	2.94
COM-Pb	6.291(5)	14.567(4)	10.09(1)	11.37%	2.81
COM-Sr	6.297(4)	14.580(3)	10.10(1)	10.56%	2.16
COM-Zn	6.286(2)	14.5600(9)	10.087(5)	10.48%	2.99

Table S2: Distances between calcium and oxygen atoms in doped and non-doped COM as obtained by means of the Rietveld refinement method.

	Distances	COM	COM-Cd	COM-Cu	COM-Pb	COM-Sr	COM-Zn
Ca1	O1	2.54(3)	2.48(2)	2.78(4)	2.72(4)	2.42(5)	2.41(2)
	O3	2.27(5)	2.45(2)	2.32(5)	2.56(3)	2.47(4)	2.44(3)
	O4	2.56(4)	2.45(2)	2.67(4)	2.48(5)	2.47(4)	2.41(2)
	O5	2.13(2)	2.33(1)	1.88(2)	1.79(3)	2.43(4)	2.39(2)
	O6	2.66(2)	2.49(1)	2.67(2)	2.68(4)	2.36(3)	2.39(2)
	O7	2.27(2)	2.42(1)	2.32(2)	2.22(3)	2.42(4)	2.48(2)
	O_{water2}	2.82(2)	2.59(1)	2.80(4)	2.75(4)	2.51(5)	2.47(3)
	$Ca1\text{-}O_{avrg.}$	2.46(3)	2.49(1)	2.46(3)	2.46(4)	2.44(4)	2.43(2)
Ca2	O1	2.37(5)	230(2)	2.30(4)	2.26(6)	2.38(5)	2.46(2)
	O2	2.37(4)	2.53(2)	2.41(4)	2.22(5)	2.29(5)	2.37(2)
	O3	2.31(4)	2.40(2)	2.29(4)	2.43(3)	2.31(5)	2.44(2)
	O6	2.67(3)	2.56(1)	2.76(3)	2.59(3)	2.53(4)	2.44(2)
	O7	2.23(2)	2.39(1)	2.28(2)	2.27(3)	2.49(4)	2.49(2)
	O8	2.41(2)	2.55(1)	2.38(2)	2.49(3)	2.48(6)	2.50(2)
	O_{water1}	2.43(2)	2.47(1)	2.50(2)	2.60(3)	2.53(4)	2.45(2)
	$Ca2\text{-}O_{avrg.}$	2.40(3)	2.42(1)	2.46(3)	2.41(5)	2.43(5)	2.45(2)