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Supplementary information

Synthesis of a novel strontium-based wide-bandgap semiconductor via X-ray photochemistry at extreme conditions.

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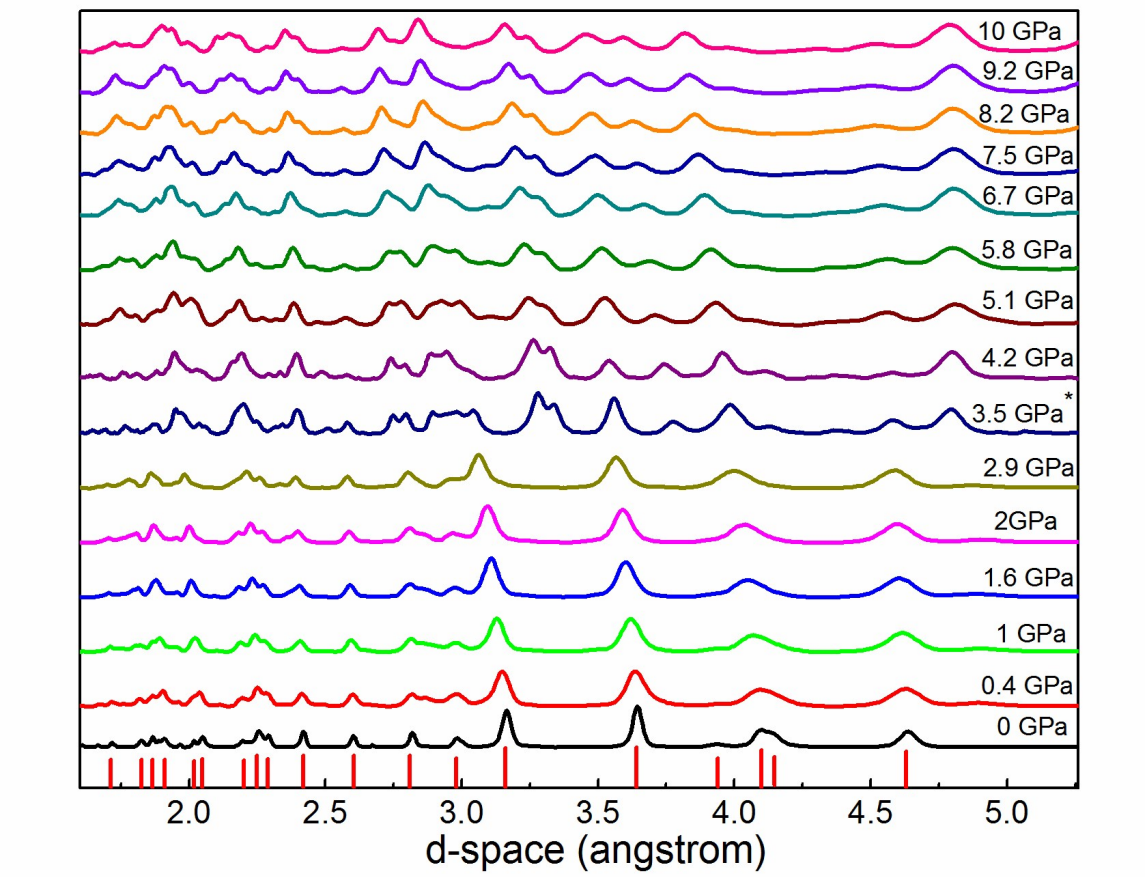

FIG. S1. XRD patterns of strontium oxalate at different pressure points (up to 10 GPa). The * symbol identifies the pressure point where the phase transition occurred. Red bars correspond to the previously-reported crystal structure of strontium oxalate (see FIG S2).

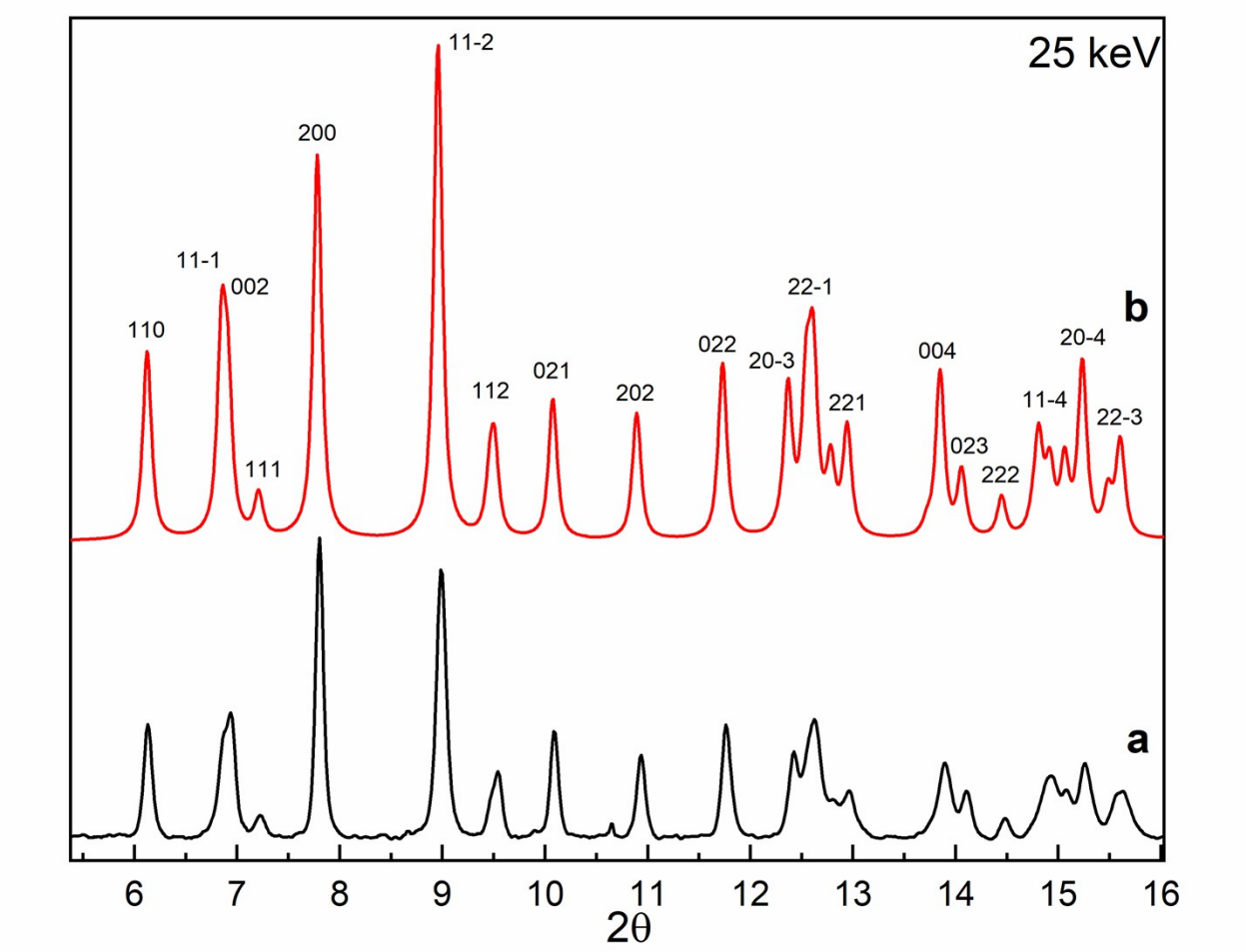

FIG. S2. XRD patterns of strontium oxalate at ambient conditions at 25 keV X-ray energy: a) experimentally obtained XRD pattern in this work, b) XRD pattern of monoclinic crystal structure of strontium oxalate[1] with a space group *C2/c* and lattice parameters: a = 7.3410 Å, b = 6.012 Å, and c = 8.267 Å. Diffraction peaks are labeled with corresponding Miller indices.

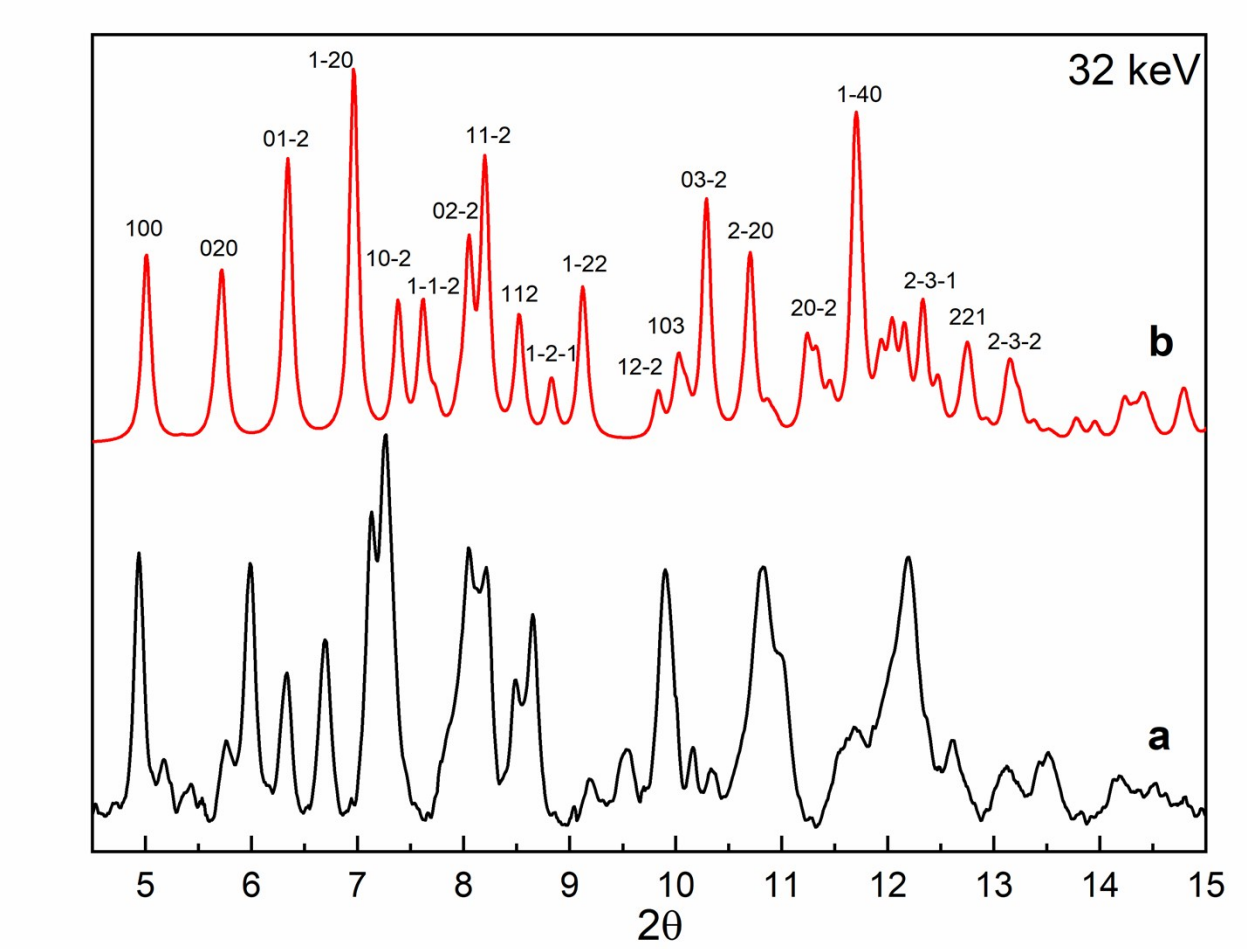

FIG. S3. XRD patterns of strontium oxalate at 4.2GPa: a) experimentally obtained XRD pattern in this work, b) XRD pattern of theoretically predicted triclinic crystal structure of SrC_2O_4 at pressure ≥ 3.5 GPa with space group *P-1* and lattice parameters a = 4.797 Å, b = 8.3763 Å, c = 8.3899 Å and α = 89.6°, β = 80.6°, γ = 87.3°. Diffraction peaks are labeled with corresponding Miller indices.

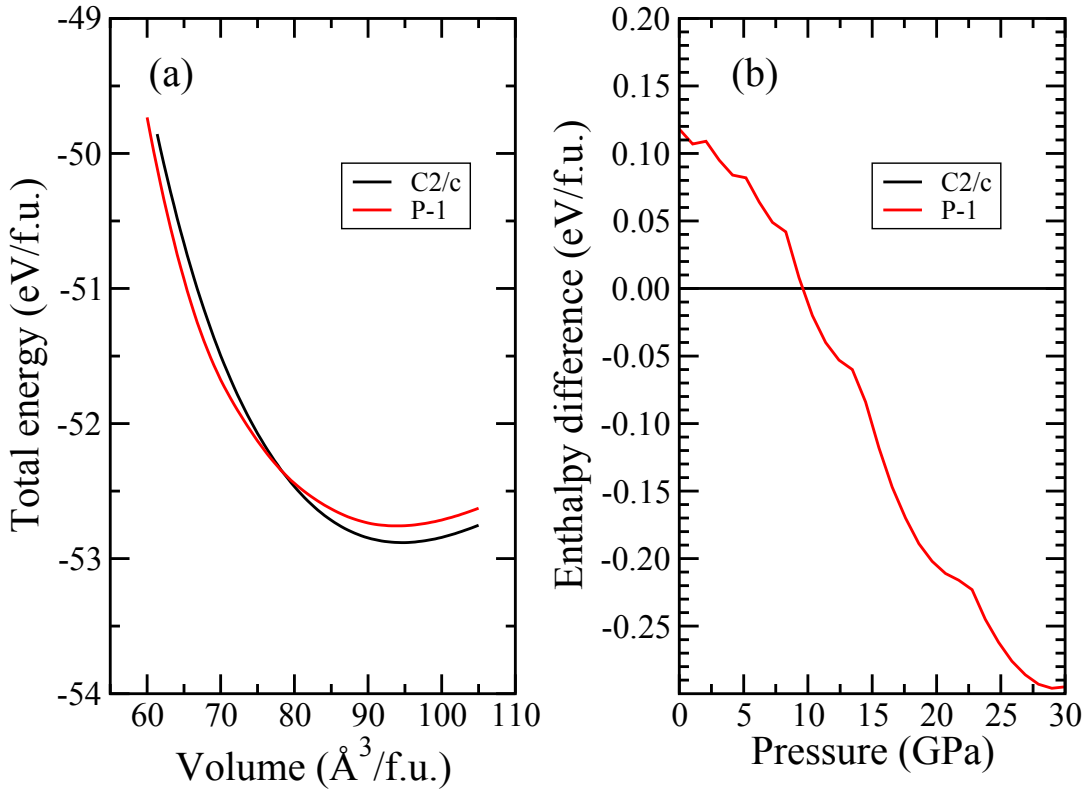

FIG. S4. Pressure-induced phase transition of SrC_2O_4 predicted from DFT calculations: (a) total energy curves and (b) enthalpy difference between the ambient SrC_2O_4 phase (space group *C2/c*, *Z*=4; back line) and the high pressure phase (space group *P-1, Z=4; red line).* The units are in eV/f.u, Å^3/f.u, and GPa for energy, volume, and pressure, respectively. The calculated transition pressure from *C2/c* to *P-1* is predicted between 9-10 GPa. However, the energy difference between *C2/c* and *P-1* phases is less than 0.12 eV/f.u. or 0.02 eV/atom, indicating the possible coexistence of both phases between 3-10 GPa as observed experimentally in XRD patterns.

Table S1. Values of synthesis pressure, thickness and optical bandgap of the DAC-synthesized samples.

Pressure, GPa	Thickness, μm	Bandgap, eV
1.03	0.038	2.45
1.98	0.033	2.46
4.00	0.034	2.46
5.36	0.033	2.49
7.13	0.027	2.53
8.20	0.036	2.53
8.89	0.030	2.50
9.80	0.040	2.52

1. D. J. Price, A. K. Powell, and P.T. Wood, *Polyhedron,* 1999, **18**, 2499.