

New shades of photochromism – yellow sodalites for the detection of blue light

Electronic supplementary information (ESI)

Hannah Byron^{a,b}, Teppo Kreivilä^a, Pauline Colinet^c, Tangui Le Bahers^{c,d}, Mika Lastusaari^{*a}.

^a Department of Chemistry, University of Turku, FI-20014 Turku, Finland.

^b University of Turku Graduate School (UTUGS), Doctoral Programme in Exact Sciences (EXACTUS), FI-20014 Turku, Finland

^c ENSL, CNRS, UCBL, Laboratoire de Chimie, UMR 5182, 46 allée d'Italie, 69634, Lyon, France

^d Institut Universitaire de France, 5 rue Descartes, 75005 Paris, France

* Corresponding author: miklas@utu.fi

Contents

| | |
|---|-----------|
| 1. XRF results and effect of potassium content on the structure and optical properties..... | 2 |
| 2. Reference XRD diffractograms of impurities and by-products in calcium-containing photochromic sodalites used in Rietveld refinement..... | 3 |
| 3. Reflectance spectra of uncoloured materials..... | 4 |
| 4. Simulated structures of Ca₂ and Na₃Ca, simulated absorbances and band transitions for all four species around V_{Cl} and oscillator strengths of all simulated transitions..... | 5 |
| 5. Unit cell parameters of calcium-containing sodalite and davyne determined by Rietveld refinement (0.27 ≤ x ≤ 1.00)..... | 6 |
| 6. Thermotenebrescence fading of the colored form and initial rise curves..... | 7 |
| 7. Emission curve of incandescent lamp for correction of fade curves..... | 9 |
| 8. XRPD and reflectance data for calcium-containing sodalites containing Cl + Br and Cl + I, x = 0.25 and x = 0.00, as well as parameters obtained by Rietveld refinement for these materials..... | 10 |
| 9. Properties of different light sources used during tenebrescence fading experiments..... | 12 |
| 10. Dose-corrected fade curves before normalization..... | 13 |
| 11. Optimized supercell structures in POSCAR format..... | 13 |
| 12. References..... | 34 |

1. XRF results and effect of potassium content on the structure and optical properties

Figure S1a shows how the calcium content measured by XRF increases in a linear fashion with x , i.e. the amount of calcium used in the synthesis. XRD data showed only very small amounts of Ca-containing by-products other than davyne (such as CaCl_2). It was assumed that almost all of the calcium observed by XRF was inside the sodalite structure.

Figure S1b shows the variation in potassium content with sample for Ca-containing sodalites made with zeolite 4A (NaAlSiO_4) and zeolite 3A ($(\text{Na,K})\text{AlSiO}_4$). Although the zeolite 4A-based materials generally contained less potassium than those made with zeolite 3A, there is some overlap in the potassium concentrations, meaning there was not a huge difference between the two starting materials. Additional potassium did not affect the position of the absorption band in the coloured form of either yellow or pink photochromism (figure S1c).

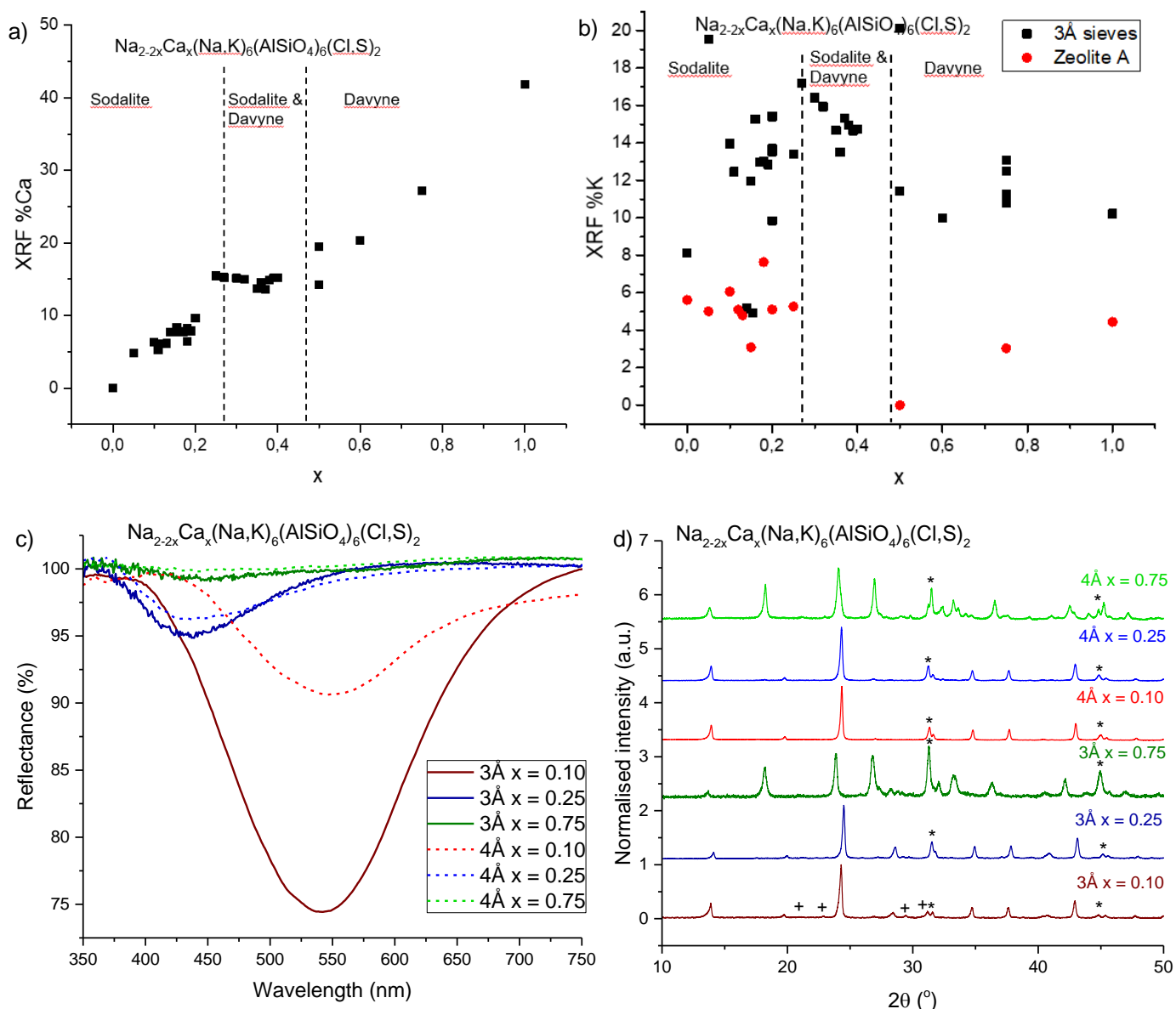


Figure S1: a) Relationship between nominal calcium content, x , and mol% Ca observed by XRF. b) Amount of potassium present in calcium-containing sodalites made with zeolite 3A and 4A. c) Reflectance of the coloured form of calcium-containing sodalites with three different values of x , made with both zeolite 3A and 4A. d) XRD diffractograms of the sodalites shown in c). NaCl impurities¹ are indicated with * and nepheline² with +. The main structures are sodalite ($x = 0.10, 0.25$)³ or davyne ($x = 0.75$)⁴.

2. Reference XRD diffractograms of impurities and by-products in calcium-containing photochromic sodalites used in Rietveld refinement

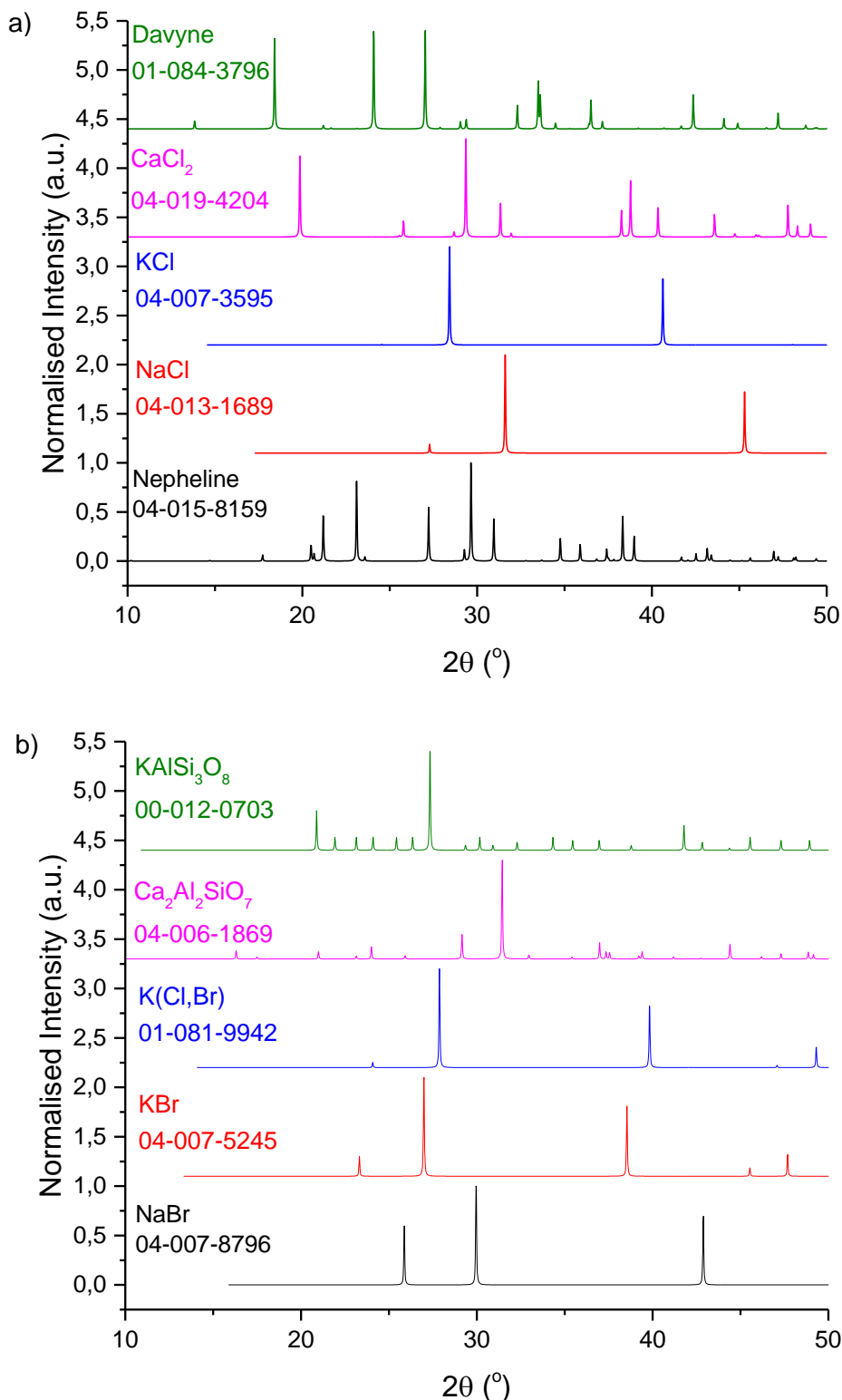


Figure S2: a) Reference diffractograms used in Rietveld refinement of $0.00 \leq x \leq 1.00$ chlorosodalites: Nepheline (PDF 04-015-8159)², NaCl (PDF 04-013-1689),¹ KCl (PDF 04-007-3595),⁷ CaCl₂ (PDF 04-019-4204),⁸ and Davyne (PDF 01-084-3796).⁴ b) Reference diffractograms used in Rietveld refinement of $x = 0.00$ and $x = 0.25$ sodalites containing Cl, Br and I: NaBr (PDF 04-007-8796),⁹ KBr (PDF 04-007-5245),¹⁰ K(Cl,Br) (PDF 01-081-9942),¹¹ Ca₂Al₂SiO₇ (PDF 04-006-1869),¹² and KAISi₃O₈ (PDF 00-012-0703).¹³

3. Reflectance spectra of uncoloured materials

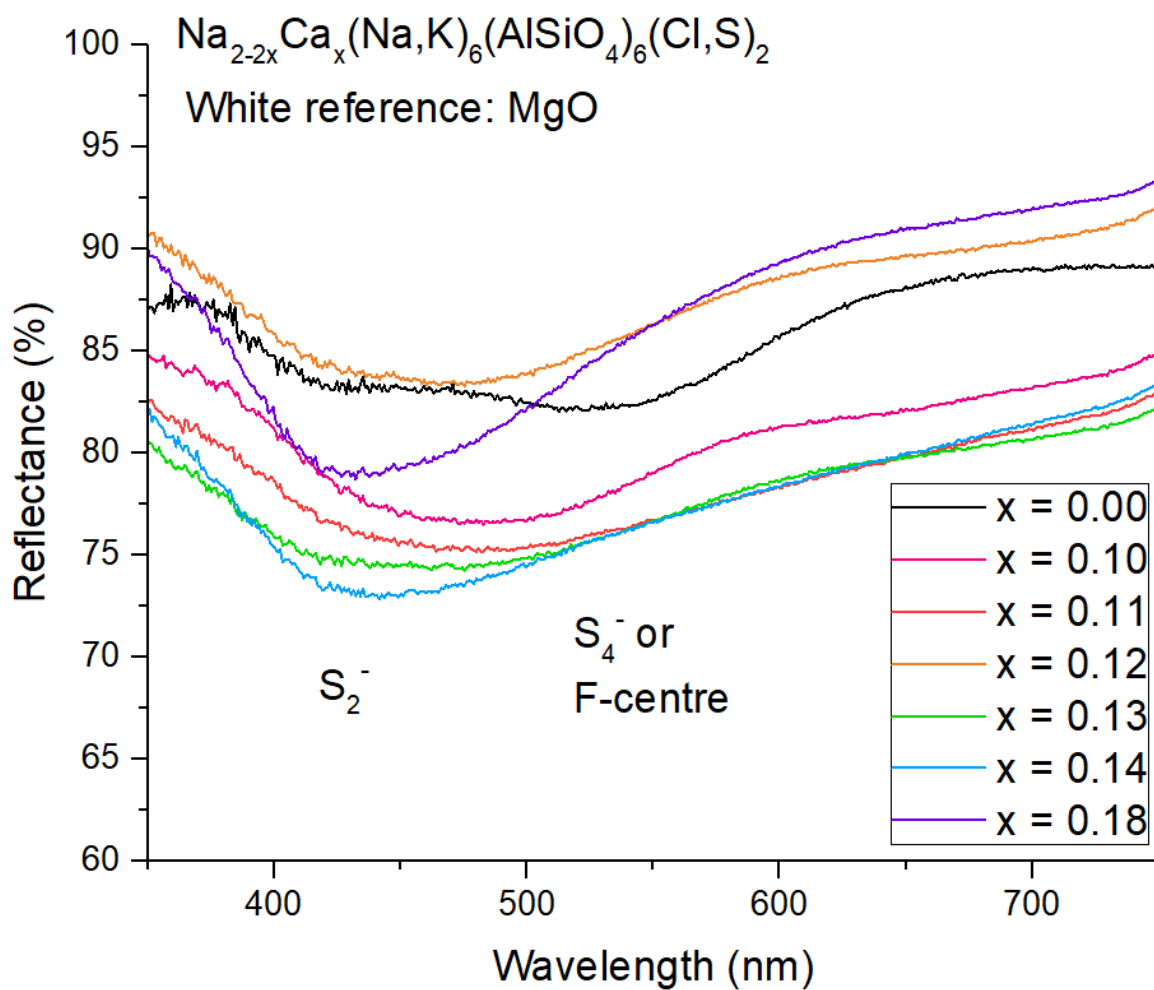


Figure S3: Reflectance spectra of photochromic sodalites before exposure to UV radiation, measured relative to a white reference of pure MgO. The suspected sulfur species responsible for the absorbances of the background colour have been indicated.^{5,6}

4. Simulated structures of Ca_2 and Na_3Ca , simulated absorbances and band transitions for all four species around V_{Cl} and oscillator strengths of all simulated transitions.

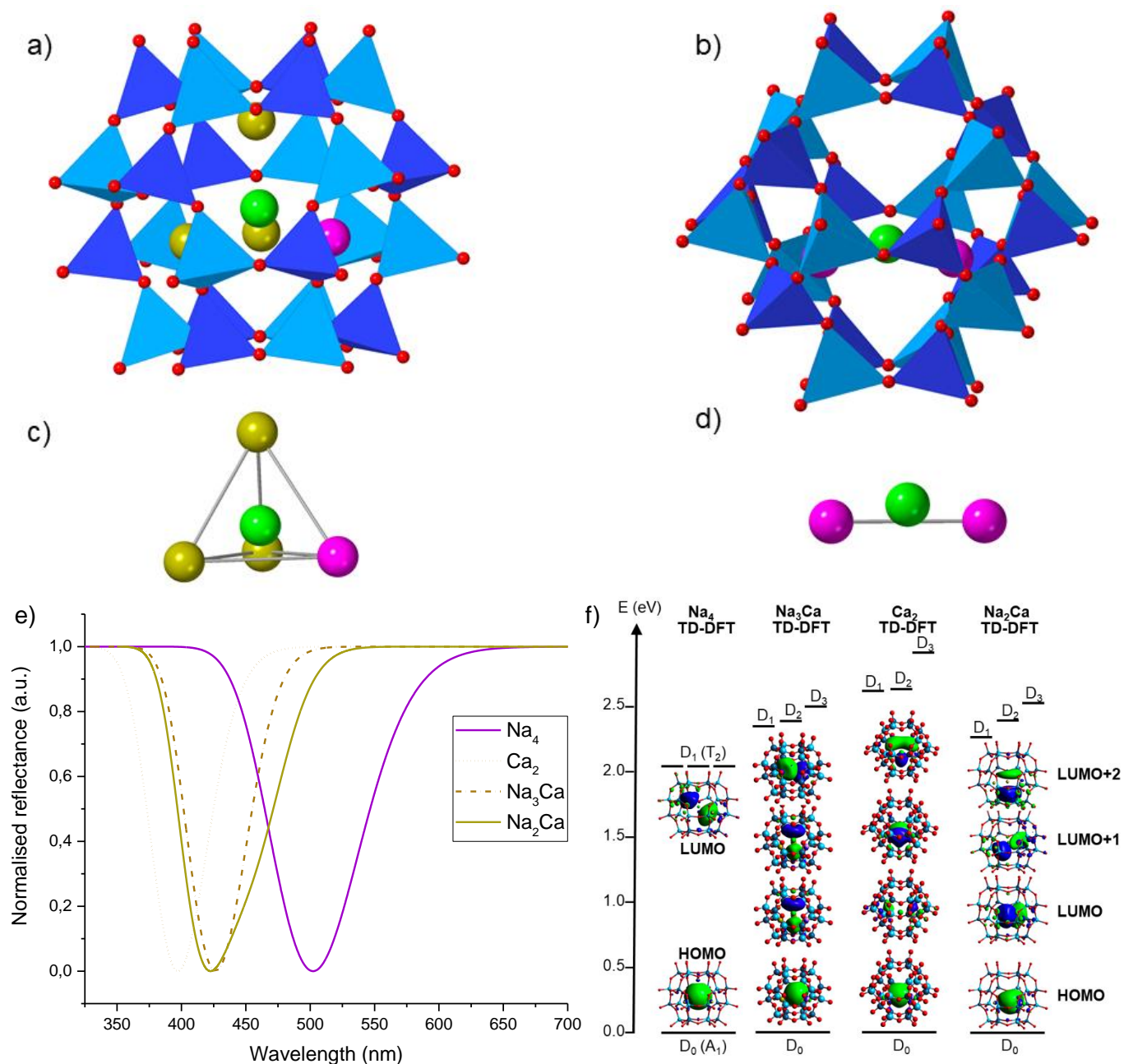


Figure S4: a-d) Structures of the system called Na_3Ca (a, c) and the defective Ca_2 (b, d) system from DFT optimized geometries showing the full beta cage (a, b) or focusing on the inside of the beta cage (c, d). Dark and light blue polyhedra surround the Si and Al atoms respectively. Red, yellow, pink and green spheres represent the oxygen, sodium and calcium atoms and the center of the cavity respectively. e) Quantum chemically calculated absorbance spectra of the colored form of the F-center formed when V_{Cl} is located in a cage containing Na_4 , Ca_2 , Na_3Ca and Na_2Ca systems. f) Energetic diagram of the three first electronic transitions for the Na_4 , Ca_2 , Na_3Ca and Na_2Ca systems computed by TD-DFT. The transitions are dominated by the HOMO to the three lowest LUMOs characters (presented as inserts). Excited states are of doublet spin-multiplicity explaining the notation D_0 , D_1 , D_2 and D_3 for ground and excited states.

Table S1: Transition energies and oscillator strengths for the F-center's transitions in the colored form of sodalites with the given species surrounding V_{Cl} .

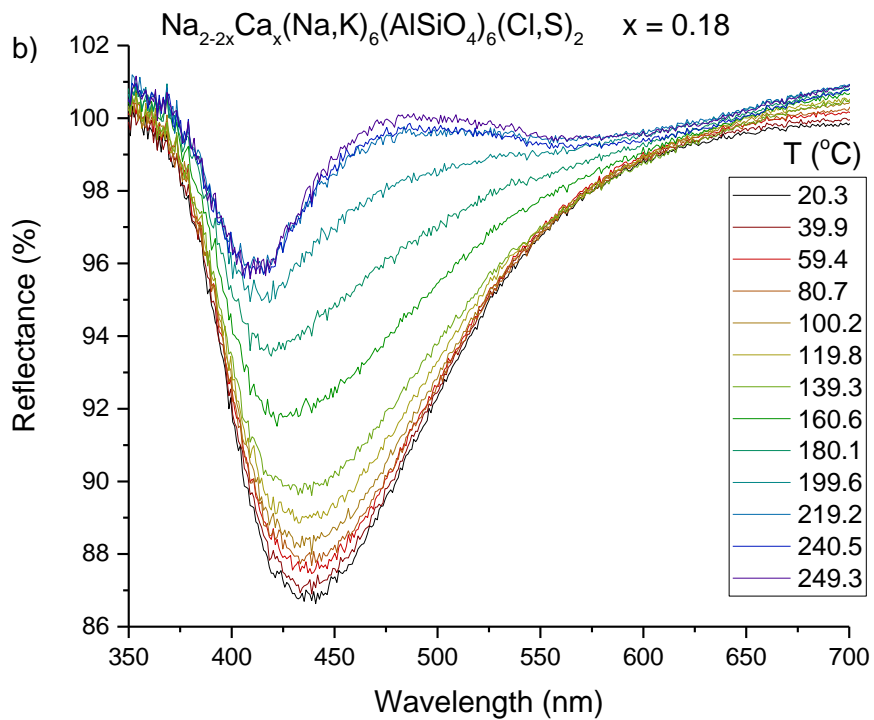
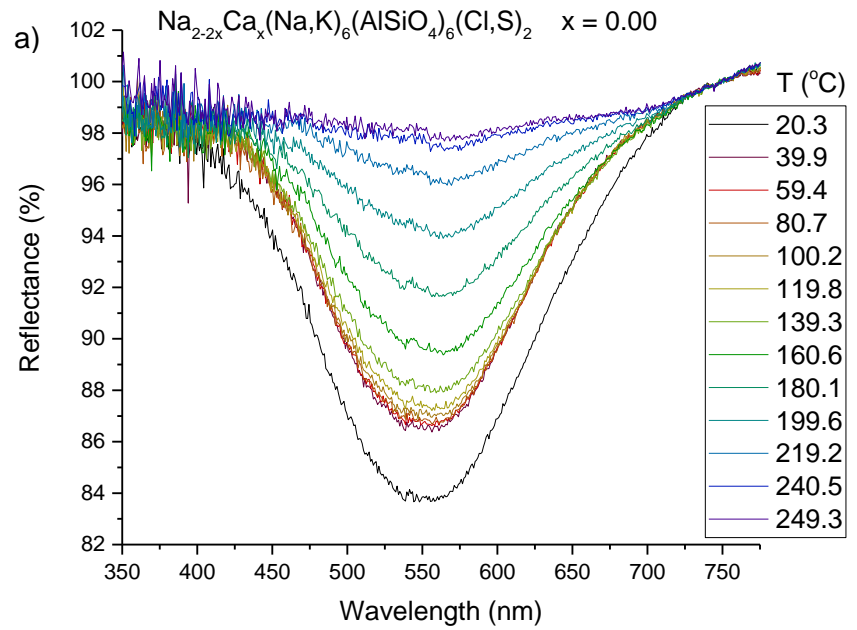
| Species surrounding V_{Cl} | Transition energy (eV) | Oscillator strength |
|------------------------------|------------------------|---------------------|
| Na ₄ | 2.4688 | 0.2154 |
| Ca ₂ | 3.0630 | 0.0825 |
| | 3.1115 | 0.1959 |
| | 3.1428 | 0.1505 |
| Na ₃ Ca | 2.8095 | 0.2207 |
| | 2.8405 | 0.2164 |
| | 2.9757 | 0.2240 |
| Na ₂ Ca | 2.6864 | 0.2233 |
| | 2.8522 | 0.1997 |
| | 3.0045 | 0.1793 |

5. Unit cell parameters of calcium-containing sodalite and davyne determined by Rietveld refinement ($0.27 \leq x \leq 1.00$)

Table S2: Unit cell parameters for sodalite and davyne phases obtained by Rietveld refinement for sodalites with $0.27 \leq x \leq 1.00$.

| x | Sodalite (%) | Sodalite a axis (Å) | Sodalite V (Å ³) | Davyne (%) | Davyne a axis (Å) | Davyne c axis (Å) | Davyne V (Å ³) |
|------|--------------|---------------------|------------------------------|------------|-------------------|-------------------|----------------------------|
| 0.27 | 52.7 | 8.913 | 708.14 | 24.6 | 12.918 | 5.318 | 778.64 |
| 0.32 | 32.9 | 8.900 | 705.01 | 47.7 | 12.919 | 5.393 | 779.55 |
| 0.35 | 31.8 | 8.912 | 707.91 | 47.6 | 12.920 | 5.394 | 779.68 |
| 0.40 | 16.5 | 8.902 | 705.53 | 62.9 | 12.911 | 5.391 | 778.25 |
| 0.50 | 0.0 | - | - | 79.2 | 12.826 | 5.378 | 766.27 |
| 0.75 | 0.0 | - | - | 74.1 | 12.877 | 5.372 | 771.51 |
| 1.00 | 0.0 | - | - | 78.0 | 12.895 | 5.313 | 773.82 |

6. Thermotenebrescence fading of the colored form and initial rise curves



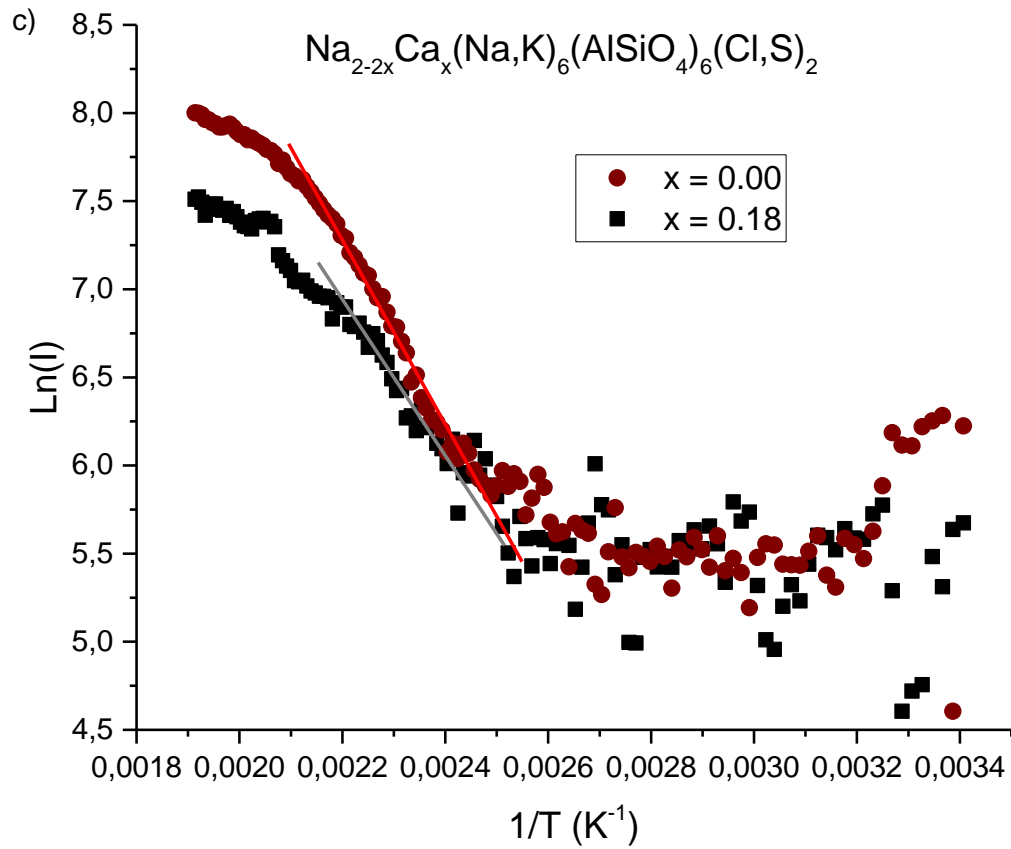


Figure S5: a) Thermotenebescence, i.e. fading of reflectance of the colored form of a calcium-free ($x = 0.00$) photochromic sodalite upon heating. b) Thermotenebescence i.e. fading of reflectance of the colored form of a calcium-containing photochromic sodalite ($x = 0.18$) upon heating. c) Initial rise curves of thermotenebescence obtained for the materials in a) and b). The regions fitted with a straight line used to obtain the trap depth with the initial rise method are indicated.¹⁴

7. Emission curve of incandescent lamp for correction of fade curves

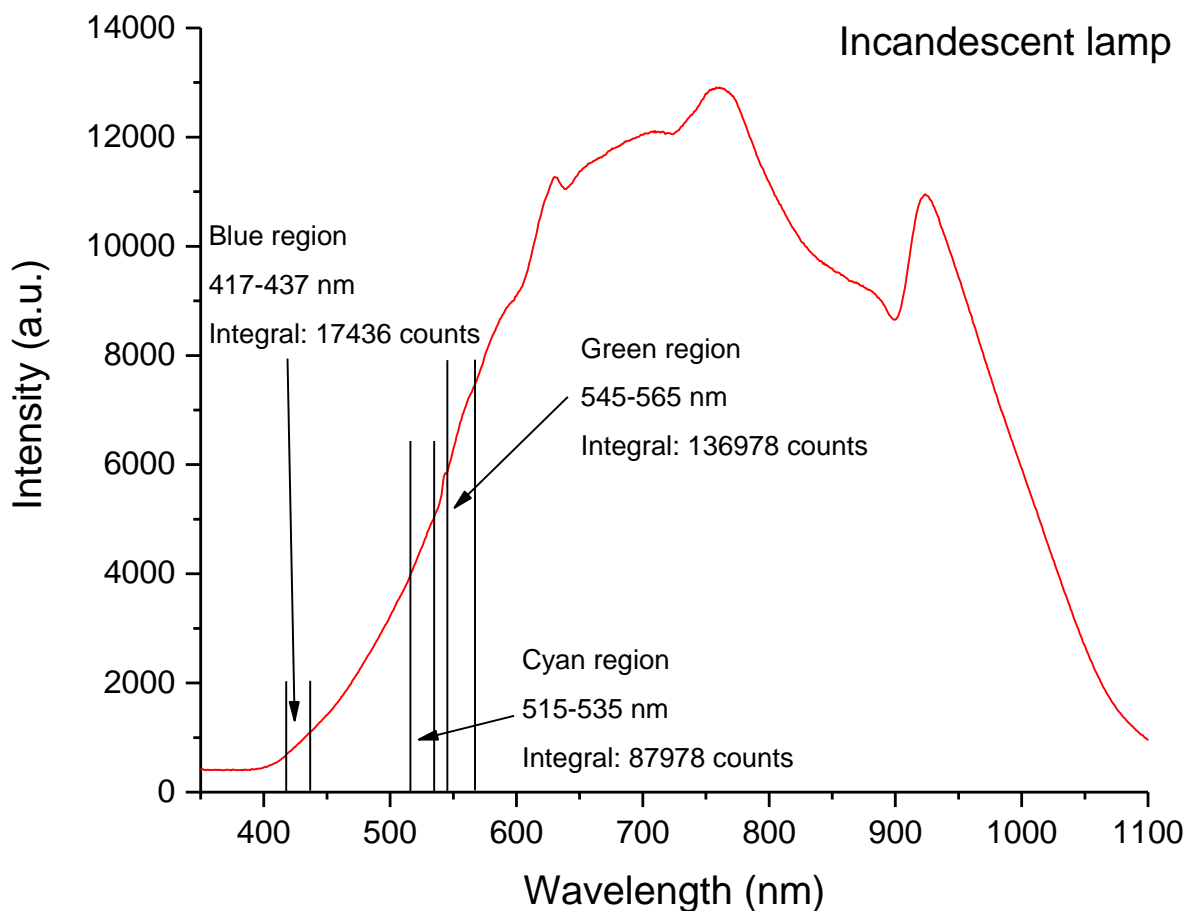


Figure S6: Emission spectrum of an incandescent lamp under which the fading of tenebrescence for $x = 0.00$ and $x = 0.18$ sodalites was measured. The intensities in the indicated regions were used to correct the fading curves with the relative irradiances of light of those wavelengths the sample was exposed to.

8. XRPD and reflectance data for calcium-containing sodalites containing Cl + Br and Cl + I, $x = 0.25$ and $x = 0.00$, as well as parameters obtained by Rietveld refinement for these materials.

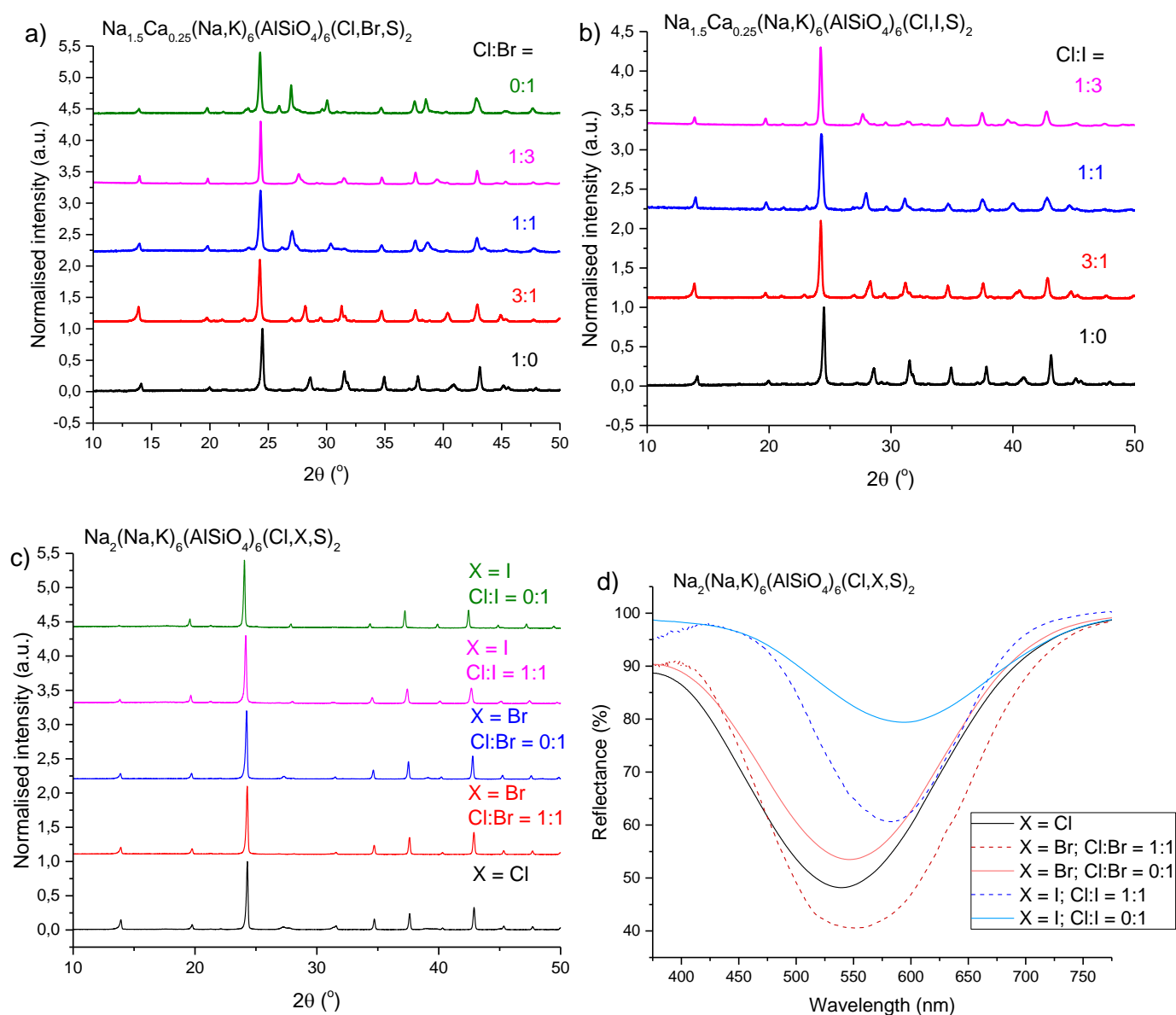


Figure S7: a) XRD diffractograms of calcium-containing photochromic sodalites with $x = 0.25$ and differing Cl:Br ratios. b) XRD diffractograms of calcium-containing photochromic sodalites with $x = 0.25$ and differing Cl:I ratios. c) XRD diffractograms of photochromic sodalites with $x = 0.00$ and differing Cl:Br and Cl:I ratios. d) Reflectance spectra of the colored forms of photochromic sodalites with $x = 0.00$ and differing Cl:Br and Cl:I ratios.

Table S3: Unit cell parameters and impurity contents of calcium-containing ($x = 0.25$) and calcium-free ($x = 0.00$) sodalites containing Cl, Br and I in varying ratios. Values obtained by Rietveld refinement.

| x | X | Cl:X | Sodalite (%) | Sodalite a axis (Å) | Sodalite V (Å ³) | NaCl (%) | KCl (%) | NaBr (%) | KBr (%) | K(Cl,Br) (%) | Nepheline (%) | Other phase (%) |
|------|------|------|--------------|---------------------|------------------------------|----------|---------|----------|---------|--------------|---------------|-----------------|
| 0.25 | - | 1:0 | 71.9 | 8.907 | 706.73 | 7.4 | 8.5 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| | Br | 3:1 | 76.3 | 8.902 | 705.50 | 8.3 | 0.0 | 0.0 | 0.0 | 0.0 | 11.5 | 0.0 |
| | | 1:1 | 76 | 8.932 | 712.58 | 8.2 | 0.0 | 0.0 | 15.7 | 0.0 | 0.0 | 0.0 |
| | | 1:3 | 69.3 | 8.930 | 712.03 | 0.0 | 0.0 | 0.0 | 0.0 | 12.5 | 0.0 | 18.2* |
| | | 0:1 | 61.4 | 8.947 | 716.22 | 0.0 | 0.0 | 0.5 | 14.7 | 0.0 | 17.0 | 6.4** |
| | I | 3:1 | 71.9 | 8.915 | 708.45 | 6.4 | 10.2 | 0.0 | 0.0 | 0.0 | 11.5 | 0.0 |
| | | 1:1 | 67.8 | 8.964 | 720.34 | 9.7 | 0.0 | 0.0 | 0.0 | 11.3 | 11.3 | 0.0 |
| | | 1:3 | 74.8 | 8.953 | 717.60 | 0.0 | 0.0 | 0.0 | 0.0 | 11.3 | 13.9 | 0.0 |
| | 0.00 | - | 1:0 | 87.1 | 8.899 | 704.62 | 6.2 | 6.6 | 0.0 | 0.0 | 0.0 | 0.0 |
| Br | | 1:1 | 99.0 | 8.917 | 708.95 | 1.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| | | 0:1 | 96.0 | 8.934 | 713.06 | 0.0 | 0.0 | 0.0 | 0.0 | 4.0 | 0.0 | 0.0 |
| I | | 1:1 | 100 | 8.957 | 718.61 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| | | 0:1 | 98.9 | 9.008 | 731.07 | 1.1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

* $\text{Ca}_2\text{Al}_2\text{SiO}_7$, PDF 04-006-1869.¹²

** KAlSi_3O_8 , PDF 00-012-0703.¹³

9. Properties of different light sources used during tenebrescence fading experiments.

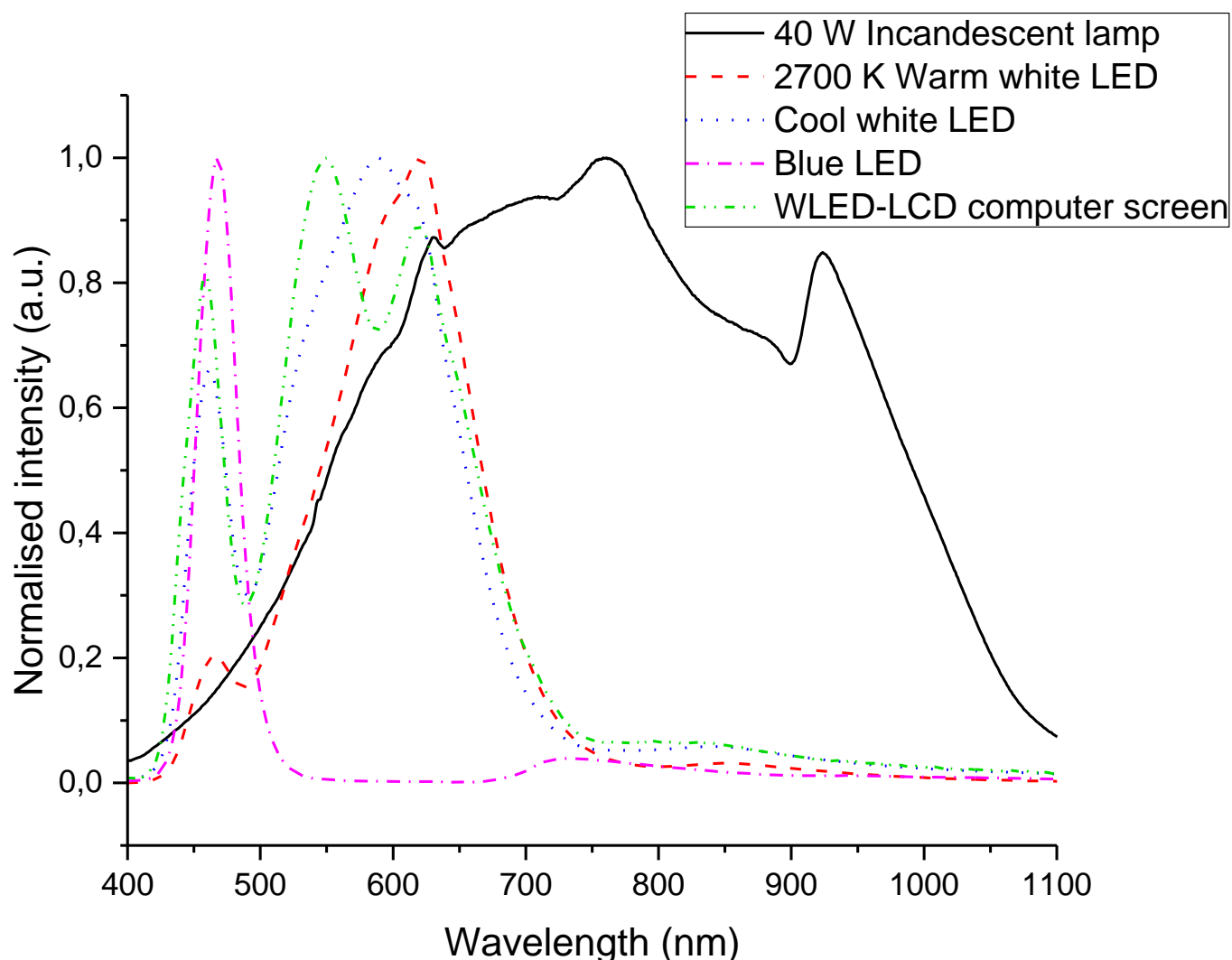


Figure S8: Normalized emission spectra of the five light sources used to measure the functionality of yellow photochromic sodalite as a blue light detector.

Table S4: Irradiances in the range 400-1050 nm for the five light sources tested, along with the proportion of blue light in the spectrum. Irradiance values were used to correct fading times for the relative doses of visible light. The blue light component is considered to be the percentage of light of wavelengths 400-480 nm compared to the entire spectrum (400-1050 nm).

| Light source | Irradiance (mW m ⁻²) | Proportion of blue light in the emission spectrum (%) |
|--------------------------|----------------------------------|---|
| 40 W Incandescent lamp | 1340 | 1.9 |
| 2700 K Warm white LED | 1800 | 4.8 |
| Cool white LED | 1240 | 12.7 |
| Blue LED | 673 | 64.5 |
| WLED-LCD computer screen | 50 | 14.9 |

10. Dose-corrected fade curves before normalization.

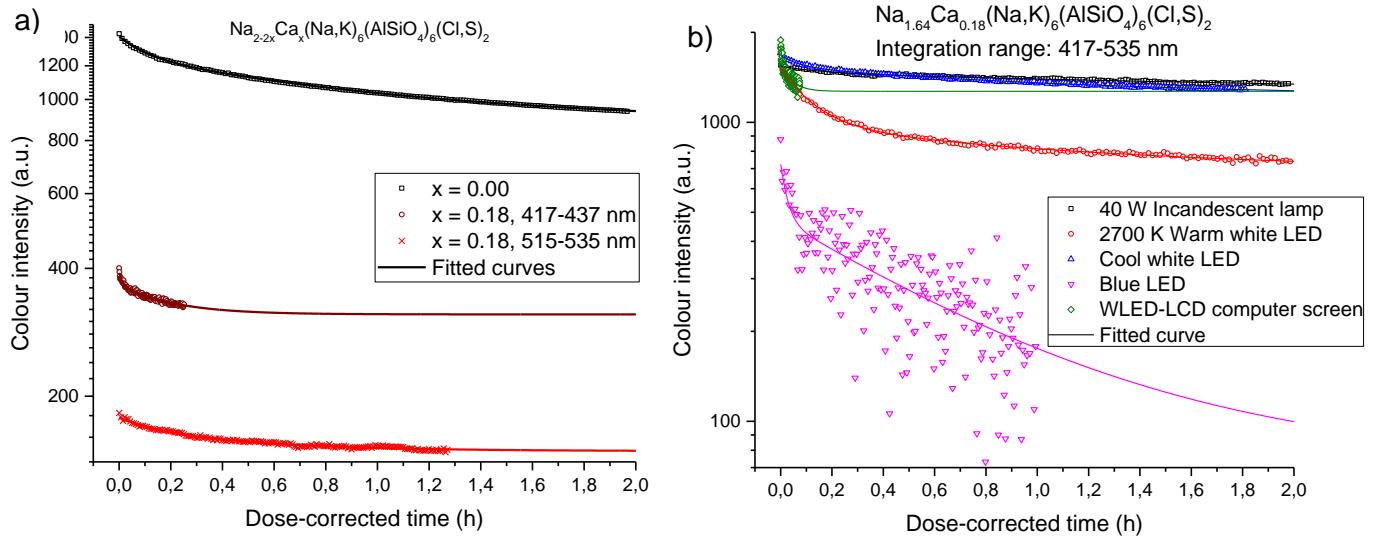


Figure S9: a) Dose-corrected coloration fade curves of $x = 0.00$ and the pink and yellow color centers in $x = 0.18$ under incandescent light before normalization, with fitted decay curves showing the predicted trend for up to two hours. b) Dose-corrected coloration fade curves of $x = 0.18$ under five different light sources before normalization, with fitted decay curves showing the predicted trend for up to two hours.

11. Optimized supercell structures in POSCAR format

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Na4
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17.65576151 0.00000000 0.00000000
0.00000000 17.65576151 0.00000000
0.00000000 0.00000000 17.65576151
Al Cl Na O Si Xx
48 15 64 192 48 1
Direct
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1.249745366913E-01 -4.999765775419E-01 2.500254180397E-01
-1.249745366913E-01 4.999765775419E-01 2.500254180397E-01
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