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Low-temperature synthesis of $CaZrTi_2O_7$ zirconolite-type materials using ceramic, coprecipitation, and sol-gel methods

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Supplemental Information

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Table S1 Synthesis conditions of ion implanted materials and the glancing angles studied by Ti K-edge GA-XANES.

Material	**Synthesis Method**	**Annealing Temperature**	**Total Annealing Time**	**Glancing Angles/Depths Studied**
$CaZrTi_2O_7$	Ceramic	1400 °C	12 days	0.8°/100 nm 3.1°/500 nm
	Coprecipitation	1200 °C	9 days	
	Sol-gel	1200 °C	9 days	

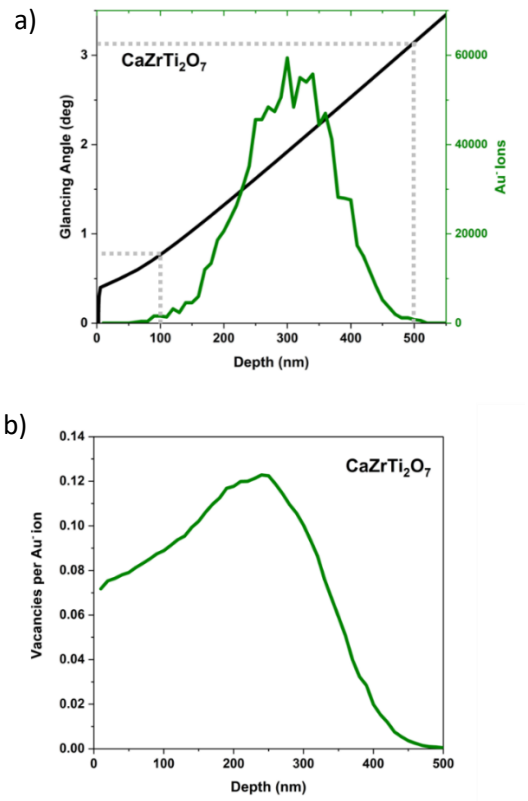

Figure S1 Ion implantation depth and X-ray attenuation depth for the $CaZrTi_2O_7$ materials are shown in **(a)**. The number of vacancies produced per Au^- ion in the $CaZrTi_2O_7$ materials is shown in **(b)**. The dotted lines present in **(a)** relate the glancing angle to the attenuation length of X-rays having an energy of 4966 eV.

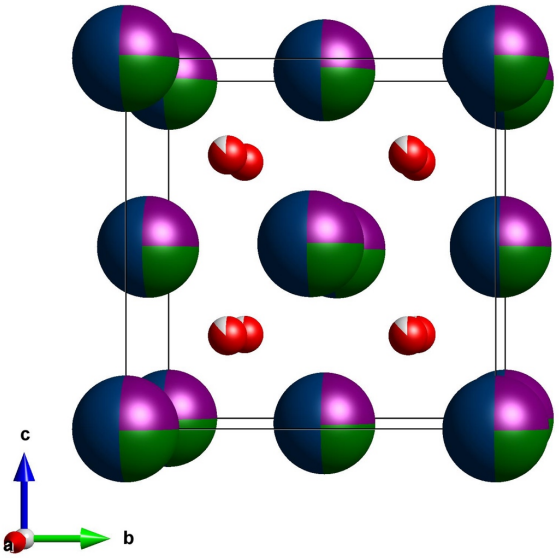

Figure S2 Skeletal representation of the defect fluorite-type structure as determined by Rietveld refinement of the diffraction pattern from the $CaZrTi_2O_7$ sample synthesized by the co-precipitation method and annealed at 700 ^oC. The purple portion of the spheres represent Ca^{2+}, the green portion of the spheres represent Zr^{4+}, the blue portion of the spheres represent Ti^{4+}, the red portion of the spheres represent O^{2-}, and the white portion of the spheres represents the random oxygen vacancies present within this structure.

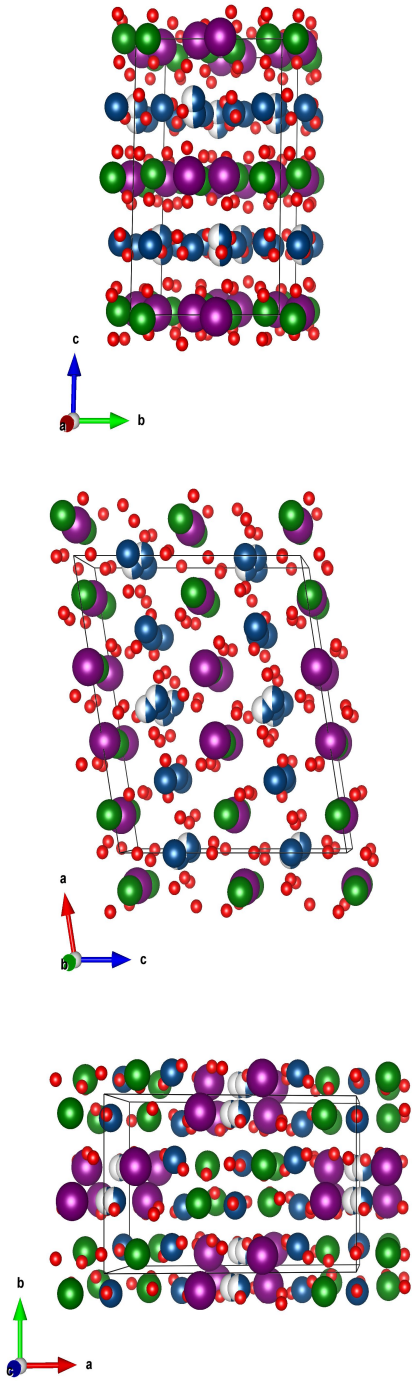

Figure S3 Skeletal representation of the zirconolite-type structure as determined by Rietveld refinement of the diffraction pattern from the $CaZrTi_2O_7$ sample synthesized by the co-precipitation method and annealed at 900 ºC. The purple spheres represent Ca^{2+}, the green spheres represent Zr^{4+}, the blue spheres represent Ti^{4+}, and the red spheres represent O^{2-}.