1. **Rapid removal of fluoride from water using core@shell and @shell nanoparticles of SiO2@ZrO2 and @ZrO2. Investigation of the mechanisms involved and impact of elemental leaching**

# Supplementary Information

# Deduction of equation (8)

|  |  |  |
| --- | --- | --- |
|  | $$\frac{mol\_{F}}{mol\_{Zr}}=\frac{\frac{m\_{F}}{AW\_{F}}}{\frac{m\_{Zr}}{AW\_{Zr}}}$$ | (1) |

|  |  |  |
| --- | --- | --- |
|  | $$\left(…\right)=\frac{\frac{ppm\_{F}. V\_{sc}}{AW\_{F}}}{\frac{ppm\_{Zr}. V\_{sc}}{AW\_{Zr}}}$$ | (2) |

|  |  |  |
| --- | --- | --- |
|  | $$\left(…\right)=\frac{\frac{ppm\_{F}}{AW\_{F}}}{\frac{ppm\_{Zr}}{AW\_{Zr}}}$$ | (3) |

|  |  |  |
| --- | --- | --- |
|  | $$\left(…\right)=\frac{ppm\_{F} . AW\_{Zr}}{ppm\_{Zr} . AW\_{F}}$$ | (4) |

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| --- | --- | --- |
|  | $$\%F=100 . \frac{mol F in ZrF\_{6}^{2-}}{mol F}$$ | (5) |

|  |  |  |
| --- | --- | --- |
|  | $$\%F=100 . 6 . \frac{ mol Zr }{mol F}$$ | (6) |

Introducing (4) in (6) yields

|  |  |  |  |
| --- | --- | --- | --- |
|  |  | $$\%F=600 . \frac{ppm\_{Zr} . AW\_{F}}{ppm\_{F} . AW\_{Zr}}$$ | (7) |

Where (7) is shown above.

Replacing ppmZr and ppmF by [Zr] and [F-] in (7) yields:

|  |  |  |
| --- | --- | --- |
|  | $$\%F=600 . \frac{\left[Zr\right] . AW\_{F}}{[F^{-}] . AW\_{Zr}}$$ | (8) |

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| 1.
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| **Figure S1.** The size distribution of solid core@shell and @shell particles in dilute dispersions.  |

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| 1. **Table S1.** The concentration of elements Na, Si and Zr (ppm) in the liquid phase measured with ICP-MS for each of the four types of material in the 17 different experiments performed in each face-centered central composite experimental
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| --- | --- |
| 1. A close up of a map  Description automatically generated
2. **Figure S2**. Modeled response surface plot showing the log concentration of leached a) Si and b) Zr as a function of pH and time.
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| 1. A close up of a map  Description automatically generated
2. **Figure S3**. Predicted individual response plots showing the log concentration of leached a) Si and b) Zr as a function of pH and time. To calculate an individual response the remaining variables were fixed to t= 24, pH = 6.5 and [F] = 6 ppm.
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