

Electronic supplementary information

Interactions between cerium dioxide nanoparticles and arsenite change their biological fate in the gastrointestinal tract of mice

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Materials and methods

Adsorption of As(III) on CeO₂ NPs in sGIFs and UPW

After temperature pre-equilibration, the solution mixture (2 mL) was incubated in the shaker (120 rpm) at 37 °C for 5 min, and then 0.8 mL of the sample was taken out for subsequent analysis. Thereafter, 2.8 mL of the simulated gastric juice was added to the remaining sample and the pH was adjusted to 2 using HCl. After 2-h incubation, 1 mL of the sample was withdrawn for further analysis. The remaining sample was mixed with 3 mL of the simulated intestinal juice and the pH of resultant mixture was adjusted to 7.5 using NaOH. After another 2-h incubation, 1 mL of the sample was pipetted out for further measurement. Similar procedure was carried out for control experiment using UPW instead of simulated GIT fluids.

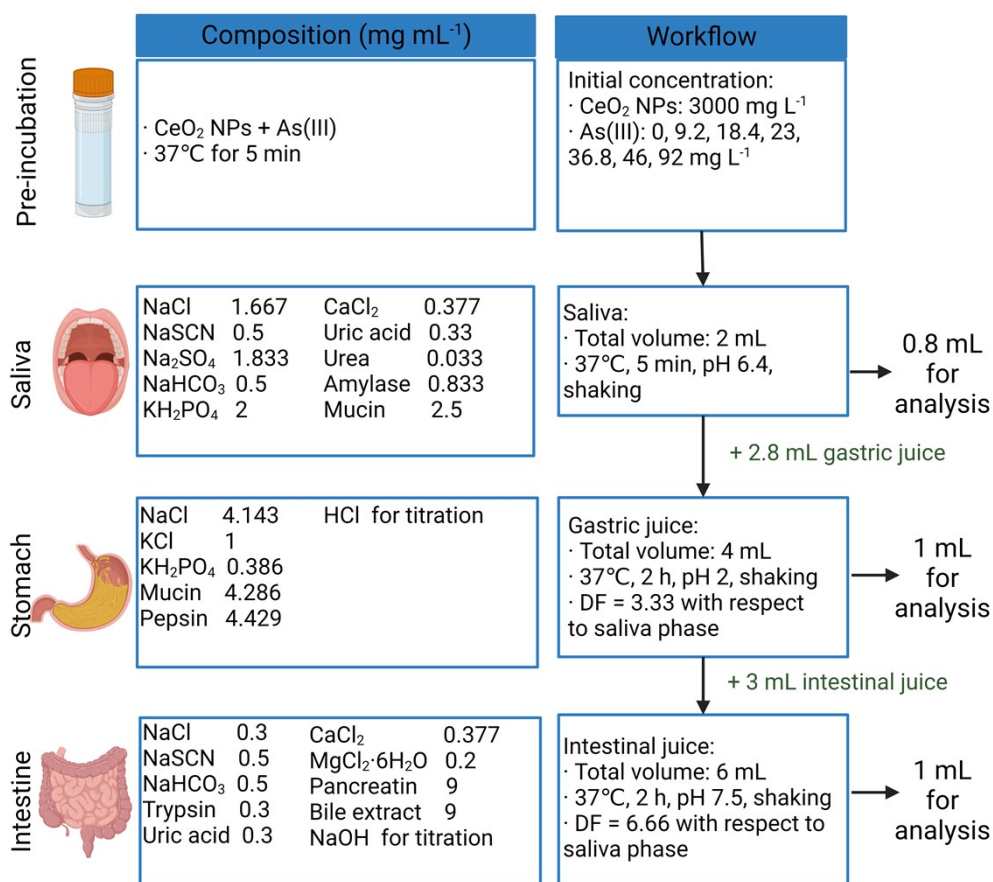


Fig. S1 Scheme of the *in vitro* GIT model including the composition of the sGIFs, workflow of experiment and the initial concentrations of CeO₂ NPs as well as As(III) in the simulated saliva.

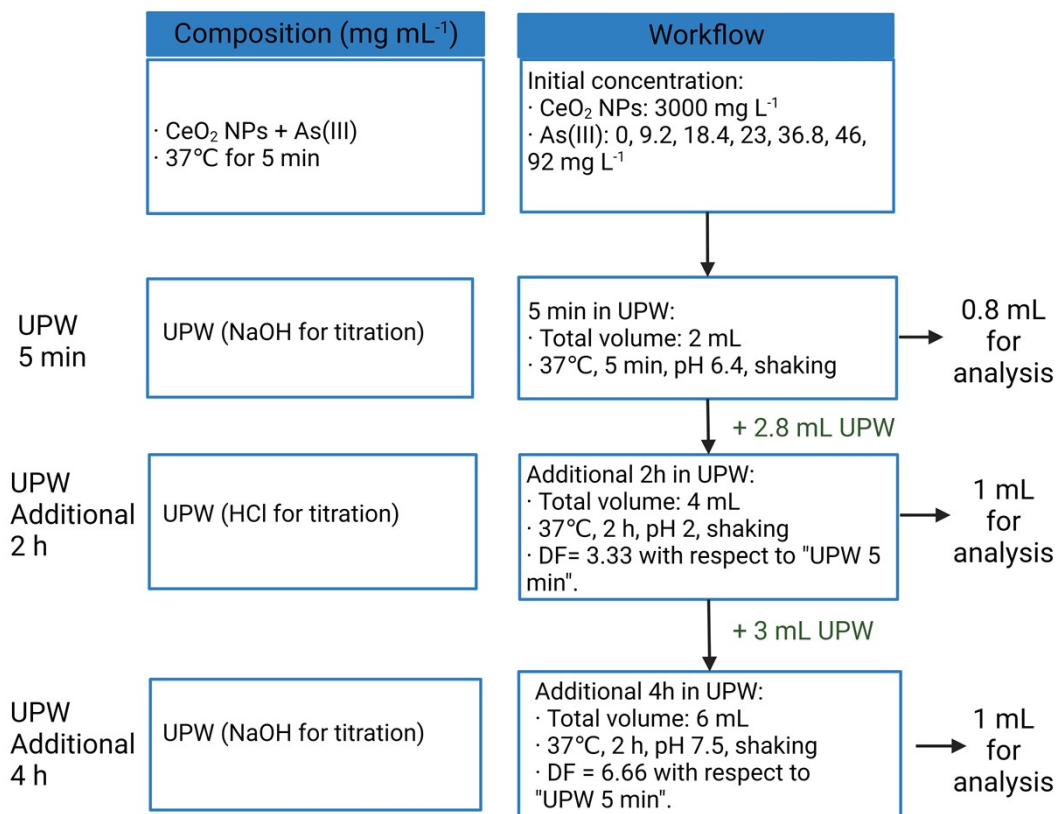


Fig. S2. Scheme of the As(III) adsorption onto CeO₂ NPs in UPW.

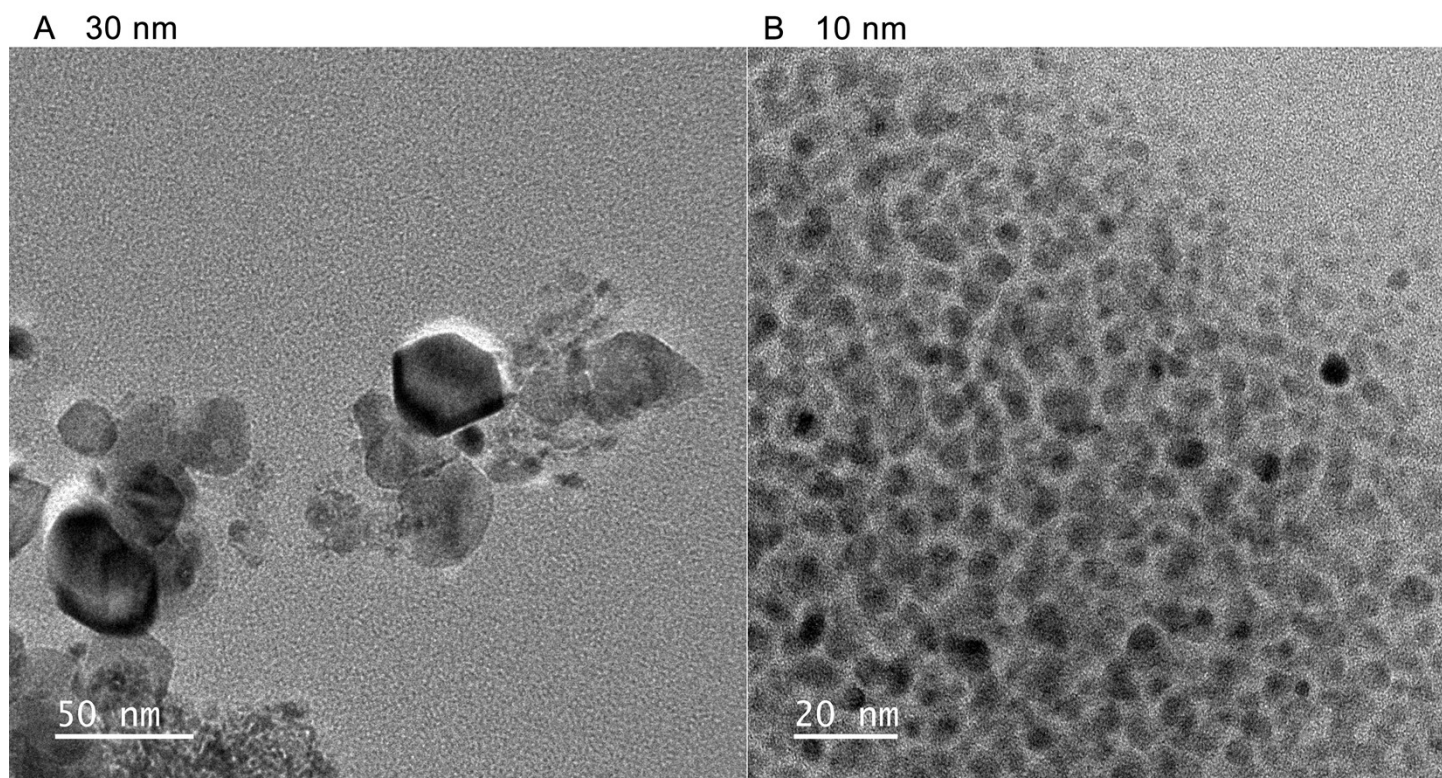


Fig. S3. The morphology of pristine (A) 30 nm CeO₂ NPs and (B) 10 nm CeO₂ NPs in ultrapure water as characterized by TEM.

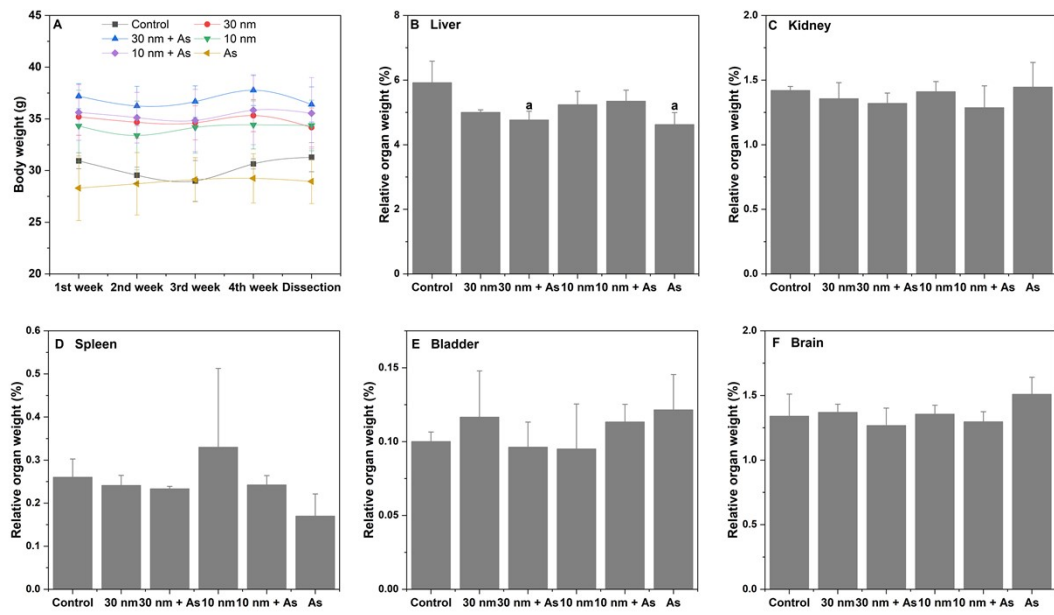


Fig. S4. The body weights (A) and relative organ weights (organ weight/body weight) (B – F) of mice (n = 4). The symbol “a” represent significant difference ($p < 0.05$) as compared with control group.

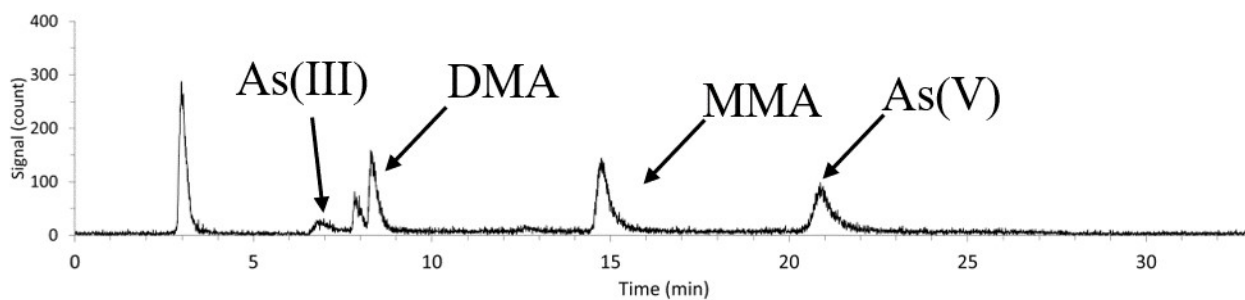


Fig. S5. LC-ICP-MS elution profile of As(III) (6.9 min), DMA (8.4 min), MMA (14.8 min) and As(V) (21.0 min) in mice liver.

Table S1. Operational parameters for ICP-MS.

Parameters	ICP-MS
RF power (W)	1400
Plasma gas flow (L min ⁻¹)	14.0
Auxiliary gas flow (L min ⁻¹)	1.0
Carrier gas flow (L min ⁻¹)	1.05
Cones	Nickel
Nebulizer and spray chamber	Micromist, Scott-type double-pass (2 °C)
Sample uptake rate (mL min ⁻¹)	0.25 – 0.35
Analysis mode	Standard
Data acquisition mode	Spectrum
Integration time	-
Measurement duration	-
Monitored elements	¹⁴⁰ Ce, ¹⁰³ Rh, ⁷⁵ As

Table S2. Operational parameters for HPLC-ICP-MS.

ICP-MS parameters		
RF power (W)	1550	
Lens voltage (V)	-12	
Nebulizer gas flow (mL min ⁻¹)	1.05	
Helium gas flow (mL min ⁻¹)	5.0	
Detection mode	Time-resolved analysis	
Integration time (ms)	400	
HPLC parameters		
Sample injection volume (μL)	20	
Flow rate of mobile phase (mL min ⁻¹)	1	
Mobile phase A	Ultrapure water	
Mobile phase B	100 mM (NH ₄) ₂ CO ₃	
Gradient elution ramp:		
Time (min)	%A	%B
0 – 3	96	4
4 – 23	60	40
24 – 33	96	4

Table S3. Recovery, LOD and LOQ of arsenic species in homogenized liver tissues of mice (n = 3).

	Homogenized liver tissue		
	Recovery (%)	LOD (ng/g)	LOQ (ng/g)
As(III)	96 ± 3	0.01	0.03
As(V)	96 ± 1	0.01	0.03
DMA	88 ± 2	0.04	0.09
MMA	99 ± 2	0.01	0.02

Table S4. Adsorption capacities (q_t) of 30 nm CeO₂ NPs for As(III) in sGIFs and UPW.

	sGIFs	q_t (mg/g)	UPW	q_t (mg/g)
Lev 1	Saliva	0.61 ± 0.16	5 min	0.58 ± 0.09
	Gastric juice	0.90 ± 0.21	Additional 2 h	2.03 ± 0.30
	Intestinal juice	1.05 ± 0.42	Additional 4 h	2.75 ± 0.40
Lev 2	Saliva	1.10 ± 0.42	5 min	0.84 ± 0.26
	Gastric juice	1.73 ± 0.33	Additional 2 h	3.85 ± 0.02
	Intestinal juice	2.04 ± 0.21	Additional 4 h	5.37 ± 0.32
Lev 3	Saliva	1.85 ± 0.05	5 min	1.04 ± 0.19
	Gastric juice	2.44 ± 0.48	Additional 2 h	4.68 ± 0.09
	Intestinal juice	3.41 ± 0.13	Additional 4 h	6.66 ± 0.43
Lev 4	Saliva	3.36 ± 0.52	5 min	1.63 ± 0.18
	Gastric juice	7.88 ± 0.50	Additional 2 h	7.62 ± 0.14
	Intestinal juice	13.11 ± 2.07	Additional 4 h	10.93 ± 0.19
Lev 5	Saliva	5.22 ± 0.17	5 min	1.94 ± 0.29
	Gastric juice	11.04 ± 0.23	Additional 2 h	9.21 ± 0.11
	Intestinal juice	17.48 ± 1.20	Additional 4 h	13.49 ± 0.12
Lev 6	Saliva	7.02 ± 0.95	5 min	4.36 ± 0.22
	Gastric juice	14.31 ± 1.13	Additional 2 h	17.47 ± 0.20
	Intestinal juice	22.69 ± 1.70	Additional 4 h	25.41 ± 0.65

Table S5. Adsorption capacities (q_t) of 10 nm CeO₂ NPs for As(III) in sGIFs and UPW.

	sGIFs	q_t (mg/g)	UPW	q_t (mg/g)
Lev 1	Saliva	2.59 ± 0.33	5 min	4.25 ± 0.76
	Gastric juice	2.41 ± 0.23	Additional 2 h	4.83 ± 0.83
	Intestinal juice	2.48 ± 0.37	Additional 4 h	4.68 ± 0.78
Lev 2	Saliva	4.99 ± 0.34	5 min	10.15 ± 1.13
	Gastric juice	5.49 ± 0.73	Additional 2 h	9.96 ± 0.63
	Intestinal juice	4.60 ± 0.28	Additional 4 h	9.75 ± 0.90
Lev 3	Saliva	6.52 ± 0.18	5 min	4.43 ± 0.58
	Gastric juice	6.92 ± 0.40	Additional 2 h	5.18 ± 0.02
	Intestinal juice	5.98 ± 0.18	Additional 4 h	4.58 ± 0.36
Lev 4	Saliva	8.64 ± 0.62	5 min	8.93 ± 0.91
	Gastric juice	8.63 ± 1.27	Additional 2 h	9.12 ± 0.99
	Intestinal juice	7.59 ± 0.60	Additional 4 h	9.29 ± 1.21
Lev 5	Saliva	11.01 ± 0.25	5 min	7.39 ± 0.92
	Gastric juice	8.31 ± 1.92	Additional 2 h	13.34 ± 1.19
	Intestinal juice	8.10 ± 0.31	Additional 4 h	24.71 ± 5.58
Lev 6	Saliva	18.24 ± 0.52	5 min	23.13 ± 3.69
	Gastric juice	12.24 ± 1.12	Additional 2 h	24.68 ± 5.95
	Intestinal juice	11.61 ± 0.12	Additional 4 h	26.14 ± 6.46

Table S6. Bioaccessibility of As(III) when it is co-existed with 30 nm CeO₂ NPs in sGIFs and UPW.

	sGIFs	As bioaccessibility (%)	UPW	As bioaccessibility (%)
Lev 1	Saliva	81.3 ± 6.0	5 min	80.8 ± 2.3
	Gastric juice	75.2 ± 5.7	Additional 2 h	36.2 ± 0.3
	Intestinal juice	70.2 ± 10.1	Additional 4 h	10.3 ± 0.2
Lev 2	Saliva	82.8 ± 6.7	5 min	86.4 ± 3.8
	Gastric juice	67.3 ± 3.3	Additional 2 h	39.1 ± 0.4
	Intestinal juice	69.3 ± 5.3	Additional 4 h	12.4 ± 0.2
Lev 3	Saliva	73.5 ± 1.1	5 min	86.5 ± 2.4
	Gastric juice	67.5 ± 4.9	Additional 2 h	40.0 ± 0.7
	Intestinal juice	60.3 ± 0.9	Additional 4 h	13.7 ± 0.3
Lev 4	Saliva	76.2 ± 3.9	5 min	87.2 ± 1.5
	Gastric juice	58.5 ± 3.1	Additional 2 h	40.9 ± 0.7
	Intestinal juice	45.5 ± 7.5	Additional 4 h	14.3 ± 0.3
Lev 5	Saliva	72.8 ± 2.5	5 min	87.9 ± 1.6
	Gastric juice	59.6 ± 2.9	Additional 2 h	42.8 ± 1.0
	Intestinal juice	47.3 ± 3.4	Additional 4 h	15.3 ± 0.3
Lev 6	Saliva	79.0 ± 2.5	5 min	89.1 ± 5.3
	Gastric juice	66.7 ± 2.6	Additional 2 h	43.8 ± 0.5
	Intestinal juice	53.1 ± 3.8	Additional 4 h	16.6 ± 0.7

Table S7. Bioaccessibility of As(III) when it is co-existed with 10 nm CeO₂ NPs in sGIFs and UPW.

	sGIT	As bioaccessibility (%)	UPW	As bioaccessibility (%)
Lev 1	Saliva	0.9 ± 0.2	5 min	0.3 ± 0.02
	Gastric juice	2.2 ± 0.1	Additional 2 h	0.9 ± 0.09
	Intestinal juice	3.6 ± 0.4	Additional 4 h	0.6 ± 0.02
Lev 2	Saliva	2.2 ± 0.2	5 min	0.6 ± 0.16
	Gastric juice	6.6 ± 1.5	Additional 2 h	4.2 ± 2.00
	Intestinal juice	9.8 ± 1.0	Additional 4 h	0.6 ± 0.23
Lev 3	Saliva	3.6 ± 0.03	5 min	0.2 ± 0.05
	Gastric juice	9.0 ± 1.1	Additional 2 h	0.4 ± 0.03
	Intestinal juice	12.5 ± 1.1	Additional 4 h	0.2 ± 0.02
Lev 4	Saliva	11.6 ± 2.0	5 min	0.2 ± 0.03
	Gastric juice	22.8 ± 2.1	Additional 2 h	1.1 ± 0.62
	Intestinal juice	27.5 ± 1.7	Additional 4 h	0.2 ± 0.02
Lev 5	Saliva	16.7 ± 0.5	5 min	1.9 ± 1.92
	Gastric juice	36.2 ± 5.4	Additional 2 h	7.7 ± 7.37
	Intestinal juice	35.2 ± 0.1	Additional 4 h	0.5 ± 0.56
Lev 6	Saliva	33.0 ± 1.4	5 min	19.3 ± 0.85
	Gastric juice	55.0 ± 3.6	Additional 2 h	21.1 ± 4.60
	Intestinal juice	56.7 ± 0.9	Additional 4 h	6.1 ± 0.06