

Article

Bio-Precipitation of Carbonate and Phosphate Minerals Induced by the Bacterium *Citrobacter freundii* ZW123 in an Anaerobic Environment

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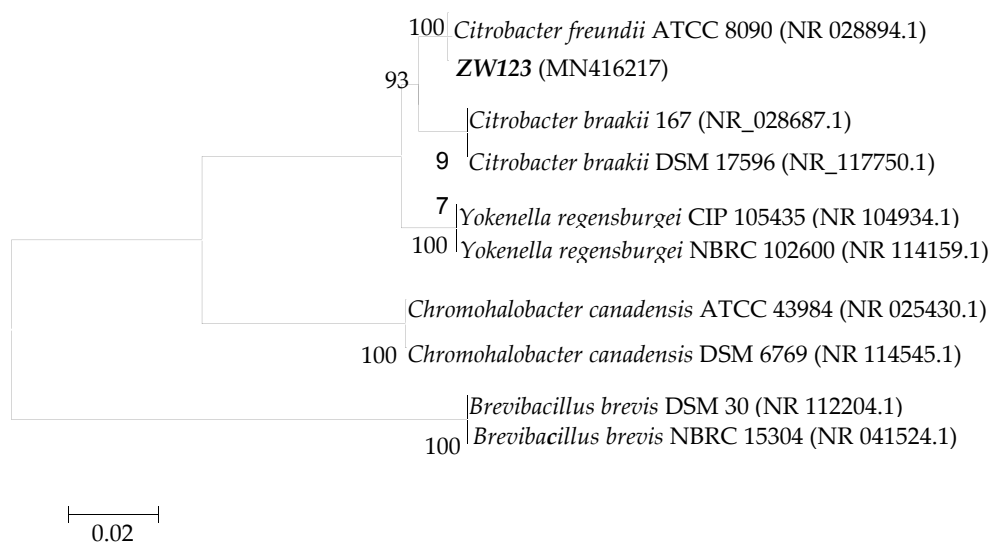
Table S1 Parameter settings of molecular dynamic simulation for adsorption of Glu onto various struvite surfaces.

Ensemble	Temperature	Time Step	Dynamics Time	Thermostat
NVT	298 K	1 fs	50 ps	Andersen

Table S2 Physiological and biochemical identification of ZW123 and *Citrobacter freundii* species

Tests	ZW123	<i>Citrobacter freundii</i> *
Gram	—	—
V-P	+	+
H ₂ S production	+	+
Amylase	—	—
Indole	—	—
Lysine decarboxylase	—	—
Ornithine decarboxylase	—	—
Bacterial motility	+	+
NH ₃ release test	+	+

Note: * Published paper of Brenner et al [57].

**Figure S1.** Phylogenetic tree of *Citrobacter freundii* ZW123 based on the sequence alignment.

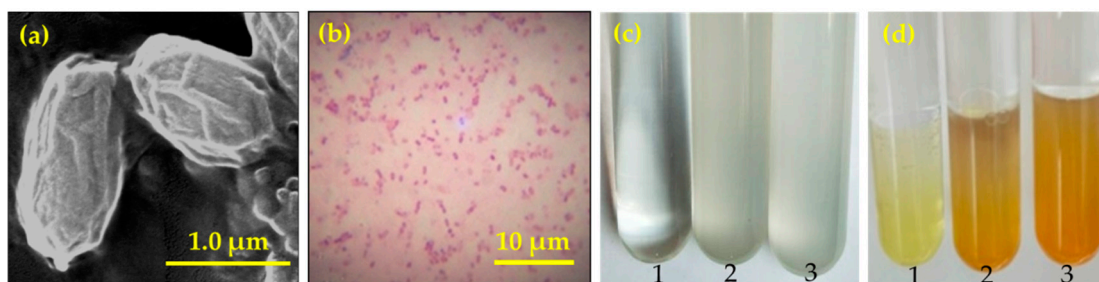


Figure S2. SEM image of *Citrobacter freundii* ZW123 bacteria (a) and Gram staining test (b) and NH₃ test (c) before adding the Nessler's reagent; d: after adding the Nessler's reagent. 1, control group; 2 and 3, experimental groups).

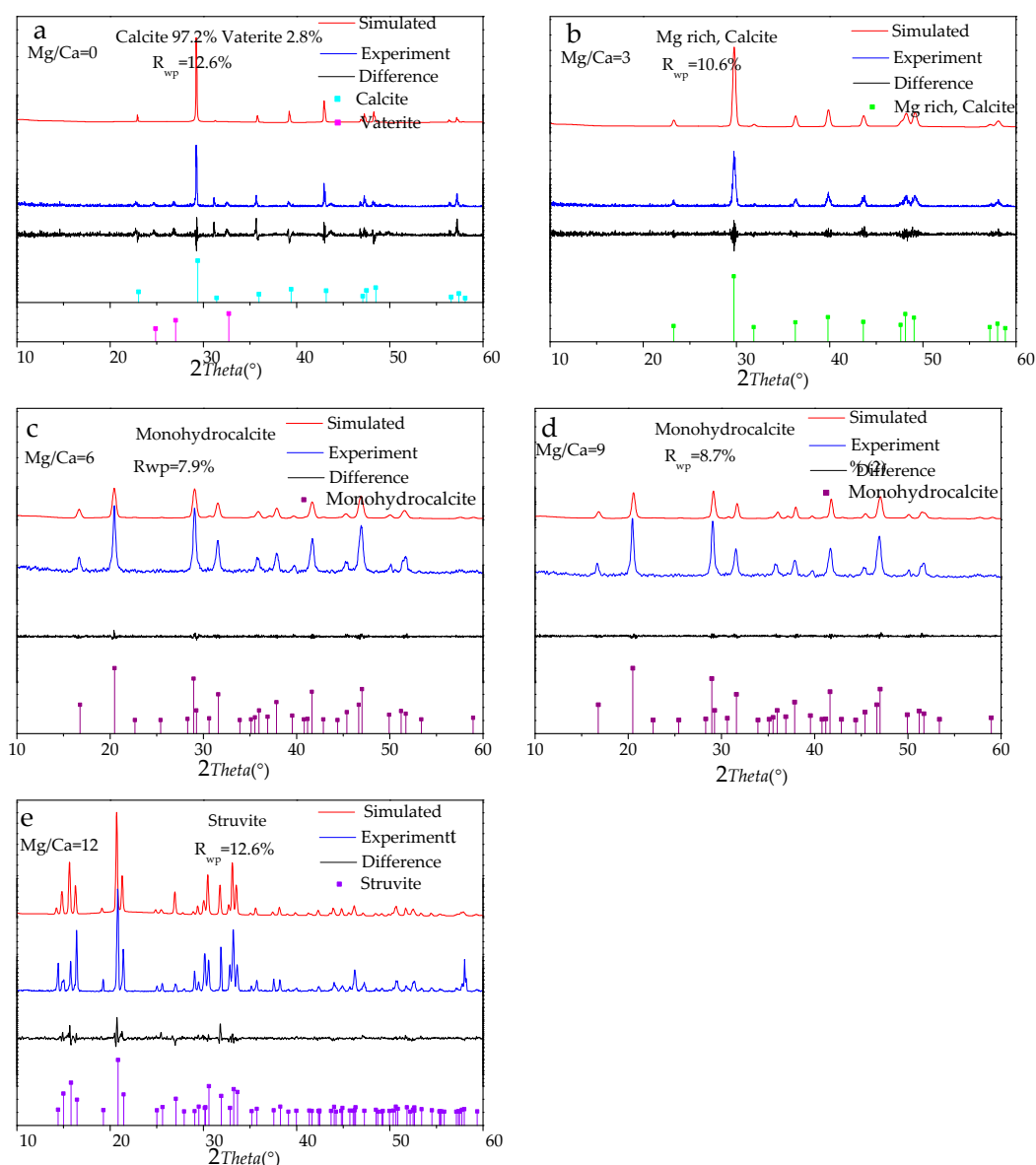


Figure S3. Rietveld refinement of XRD data at Mg/Ca molar ratio 0 (a), 3 (b), 6 (c), 9 (d) and 12 (e).

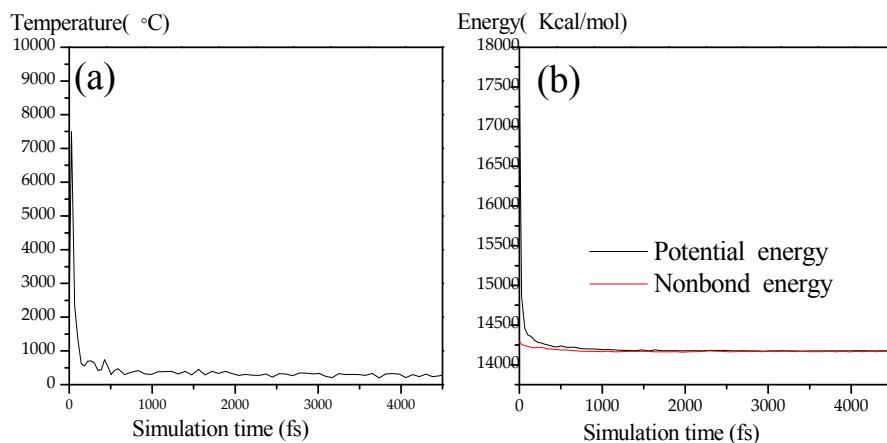


Figure S4. Molecular dynamics simulation of adsorption of Glu onto crystal: **a**: temperature fluctuation of the adsorption of Glu onto (111) faces; **b**: energy fluctuation of the adsorption of Glu onto (111) faces.



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