

## Selective ion adsorption of Prussian blue nanoparticle: A 3D-RISM study

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Diffusion of the radionuclides is a serious concern to give damage to living beings. In 2011, the reactor of the Fukushima Daiichi Nuclear Power Plant melted down and released more than 600,000 TBq of radioactive nuclides including  $^{137}\text{Cs}$  into environment.[1] A radioactive Cs,  $^{137}\text{Cs}$ , has attracted a lot of attention due to its high radioactivity and long half-life. Therefore, an efficient material for the removal of Cs from environment is highly anticipated. Prussian blue (PB),  $\text{Fe}_7(\text{CN})_{18}$ , is one of the candidates, which is known as a highly selective adsorbent of  $\text{Cs}^+$ . [2]

The three-dimensional reference interaction site-model (3D-RISM) theory is a useful tool to investigate the selective ion adsorption. This theory is a statistical mechanics theory of molecular liquids, which provides the spatial distribution of solvent species such as ions and water. The validity of the theory has been demonstrated by numerous applications to biophysical and biochemical phenomena including the selective ion binding of biomolecule.[3] Recently, we have applied the 3D-RISM theory to investigate the distinct configuration of cations in the KcsA potassium channel.[4] The results showed a perfect agreement with experimental observations.

In the present study, we applied the 3D-RISM theory to investigate the molecular mechanism of the selective ion adsorption of PB. In Figure 1, the  $\text{Cs}^+$  distribution inside a PB nanoparticle is depicted. The conspicuous distribution is found in the cage of the PB lattice, which indicates high affinity of PB to  $\text{Cs}^+$ . We also evaluated the distribution of other alkali metal ions ( $\text{Li}^+$ ,  $\text{K}^+$ , and  $\text{Na}^+$ ) and compared the results with that of  $\text{Cs}^+$ . The details of the results are presented in the poster session.

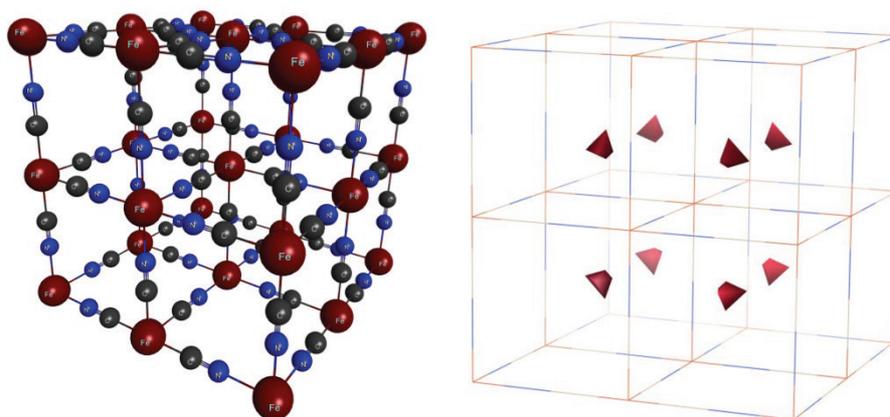


Figure 1: Structure of PB nanoparticle (left) and isosurface plot of  $\text{Cs}^+$  distribution (right).

[1] X. Liu et al., *Bioresource Tech*, **160** (2014) 142-149

[2] H. Fujita et al., *Adsorption*, **20** (2014) 905-914

[3] N. Yoshida et al., *J. Phys. Chem. B.*, **113** (2009) 873-886

[4] S. Phongphanphanee et al., *J. Mol. Liquids*, **200** (2014) 52-58