Adsorption of GMP and dGMP nucleotides onto Na-montmorillonite using molecular dynamics simulation

PAULINE BACLE[1], SEBASTIEN LE CROM[1], VIRGINIE MARRY[1]

[1]PHENIX UMR 8234, Sorbonne Université, Paris 75005, France

The concentration of prebiotic organic building blocks may have promoted the formation of biopolymers in the environment of the early Earth. Therefore, the adsorption of of RNA and DNA monomers (nucleotides) on minerals that were abundant in the early Earth environment has been largely investigated both theoretically[1,2] and experimentally[3,4]. In particular, adsorption studies on swelling and non-swelling clays have shown that DNA monomers adsorb much more strongly than RNA monomers[4]. Yet, the only difference between deoxyribonucleotides and ribonucleotides is the hydroxyl group on the 2' carbon of the deoxynucleotide's pentose which is reduced to just a hydrogen atom. Moreover, experimental results showed that even if adsorption of nucleotides occurs primarly on the lateral surfaces of clay particles, adsorption on the basal surfaces might happen at low pH for swelling clays, which are negatively charged.

In the present study, we present molecular dynamics simulations of the adsorption of both guanosine monophosphate GMP and its deoxy- version, dGMP, on the basal surface of montmorillonite. For dGMP, two adsorption configurations were found whereas only one stable configuration was observed for GMP. The relative stabilities of these two adsorbed configurations were then further studied by Metadynamics simulations. The role of the presence of the hydroxyl group was also investigated. Our results were discussed in the light of experimental data obtained with similar systems[4].

[1] Mignon P. et al (2009 J. Phys. Chem. C, 113, 13741-13749.
[2] Swadling J. et al (2010) J. Am. Chem. Soc, 132, 13750-13764.
[3] Feuillie C. et al(2013). Geochim. Cosmochim. Acta, 120, 97-108.
[4] Peidreira-Segade U. et al (2016) Geochim. Cosmochim. Acta, 176, 81-95.