The crucial role of water for covalent immobilisation of DNA onto alumina surface: a first principles investigation

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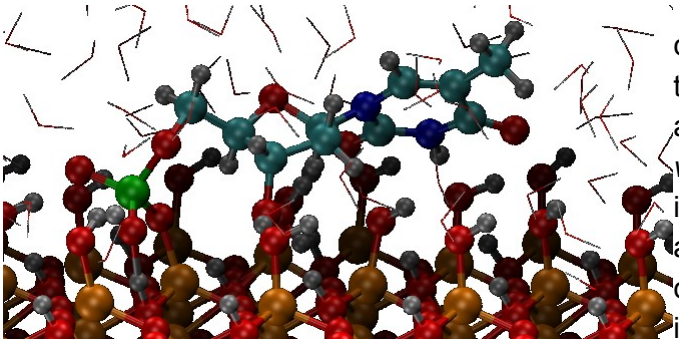
Beside its crucial biological function as genetic information carrier, DNA is a promising building block for the elaboration of new materials due to its properties of self-organization, molecular recognition, or ease of chemical modifications. However, its integration into a technological device requires its immobilization onto a relevant surface in a controlled and reproducible way. With the notable exception of the well-controlled thiol – gold grafting[1], this immobilization generally requires complex multistep protocols introducing variability.

As an alternative, we have recently used a combination of experimental and computational methods to show that a nucleotide, the (deoxy-)thymidine mono-phosphate (dTMP), can covalently bonds to aluminum oxide surfaces[2]. Still the exact nature of the DNA attachment to the surface remains elusive from these experiments.



In this contribution, we use van der Waals corrected Density Functional Theory[3] calculations to describe the bonding of the dTMP to an alumina surface. In a first time we investigate *in vacuo* how the different polar groups drive this interaction. In a second time, we add a large amount of water molecules to produce models closer to realistic conditions and study how the interaction evolves. Within this model, solvation of both dTMP and reaction products are taken into account. We demonstrate that *in vacuo* dTMP exposure leads to a physisorbed state, the dTMP lying flat on the surface. On the contrary, water solvation thermodynamically favors surface exchange reactions promoting covalent grafting.

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3. Vydrov O.A., van Voorhis T., *Nonlocal van der Waals density functional: The simpler the better*, Journal of Chemical Physics 133, 244103, 2010.