DFT Study of a Relaxed Amino Acid, Glutamine, on TiO_2 Surfaces

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1. INTRODUCTION:

Linking inorganic systems with organic ones is a highly important avenue for finding new drugs and treatment methods. Several amino acids have roles in supporting cancer growth, and one of the inorganic materials that can show antitumor properties is titanium dioxide. In this study we choose anatase as titanium dioxide crystal modification and an amino acid - Glutamine (L) molecule.

The aim of this research was to investigate potential interaction of TiO_2 slab and a Glutamine (L) amino acid molecule, which would make a significant contribution to the study of antitumor properties of TiO_2 for particular tumor cell lines whose proliferation is not possible without Glutamine.

2. METHODS:

Density functional theory (DFT) method with:

1) exchange-correlation Local-density approximation (LDA) with Perdew–Zunger (PZ) correlation functional (CRYSTAL17 code);

2) Generalised gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) functional implemented in Quantum Espresso code.

We first locally optimized 2D-slab structures of undoped and doped anatase (001 and 101 surfaces), then similarly optimized a single molecule of glutamine in vacuum. We placed the pre-optimized glutamine molecule in various orientations (rotations of 0°, 90° and 180° relative to the previous position of a molecule) to the central position onto the relaxed substrate surfaces (3 x 3 supercell slabs), and then performed ab initio relaxations of the molecule on the substrate slabs.

3. RESULTS:

The results suggest that the particular conformation of a Glutamine (L) molecule on pristine anatase slab 001 and 101 surfaces show presence of an interaction between molecule and a slab, contributing to the lowest total energy of system, for both types of surfaces (Figures 1 and 2, Table 1).

The same conformation of Glutamine (L) molecule has not showed such deformation in interaction with Au doped 001 anatase surface (Figure 3 and Table 1).

Table 1

Surface type		Energy [Ry]
001	Single Glutamine (L) molecule	−206.0196618296
	Pristine Anatase Slab	−3297.6649479915
	Slab + Glutamine (L)	−3504.0150932361
101	Single Glutamine (L) molecule	−206.0196618296
	Pristine Anatase Slab	−3296.4745311656
	Slab + Glutamine (L)	−3502.8226042723
Au doped 001	Single Glutamine (L) molecule	−206.0196618296
	Au doped Anatase 001 Slab	−3293.4406901053
	Au doped Anatase 001 Slab+ Gln	−3499.7504625409

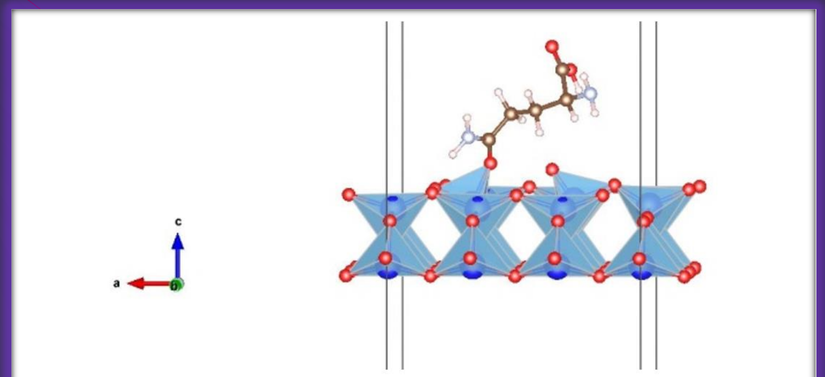

Figure 1. An interaction of Glutamine (L) molecule and relaxed pristine anatase slab surface 001 after optimization, visualized by VESTA program.

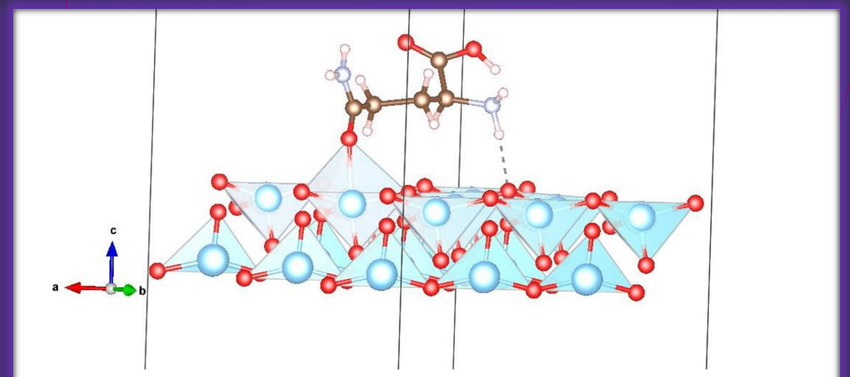

Figure 2. An interaction of Glutamine (L) molecule and relaxed pristine anatase slab surface 101 after optimization, visualized by VESTA program.

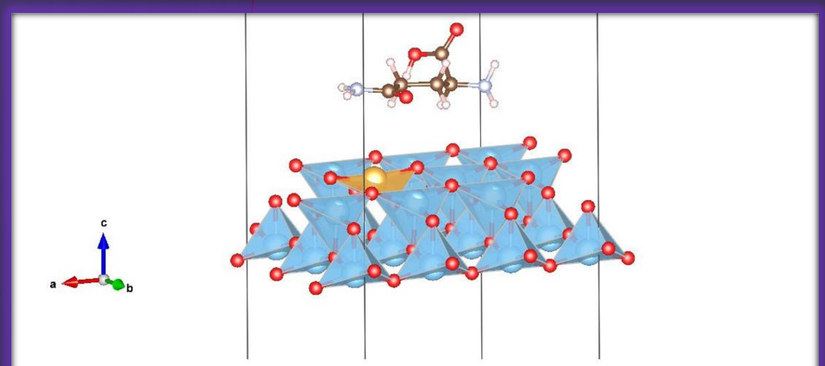

Figure 3. Optimized structure of Glutamine (L) molecule on Au doped anatase slab surface 001, visualized by VESTA program.

4. CONCLUSIONS AND FUTURE GOALS:

Comparison of the optimized conformations, electronic structure and properties of the amino acid in vacuum and on the surface, yield useful insights into various biological processes.

In order to determine the energy of deformation and adsorption, additional calculations for presented interactions will be performed.

In the future we will investigate potential significant interactions with other Glutamine (L) conformations and with another substrate dopants.