

Figure S1. Schematic diagram showing the chemical coupling steps for immobilization of the aptamer, on the SiO₂ surface. [A] Coupling of amine at the 5'-amine of the MC-LR aptamer with the N-hydroxysuccinimide (NHS) Ester group connected with the dibenzocyclooctyne (DBCO). [B] Result from the coupling reaction in [A]. [C] Molecule used for surface functionalization, 3-(Azidopropyl) triethoxysilane (AzPTES). [D] Typical result of AzPTES reacted with a glass/SiO₂ surface. [E] Final result of the aptamer attached to the surface following click chemistry of the DBCO-modified DNA to the azido group.

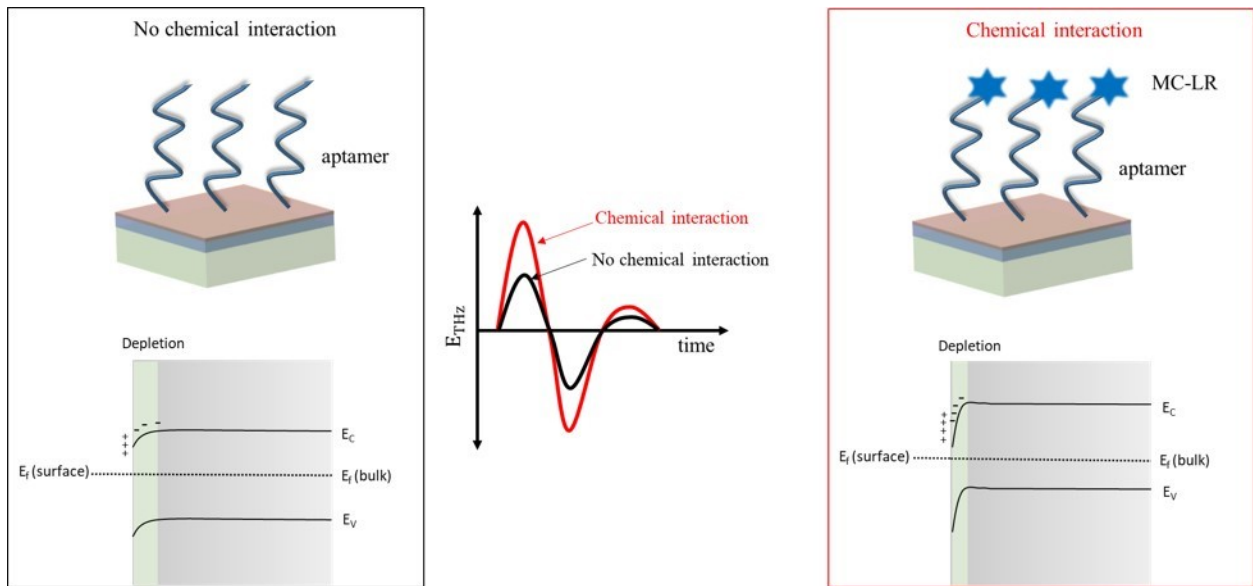


Figure S2. Schematic diagram showing the working principle of the TCM system. When the MC-LR binds to the immobilized aptamer, both valence and conduction bands at the interface between Si and SiO₂ would be re-bent to re-stabilize the chemical potential, Fermi level, at the surface. Consequently, the built-in electric field is changed, and thus, the THz amplitude is changed.

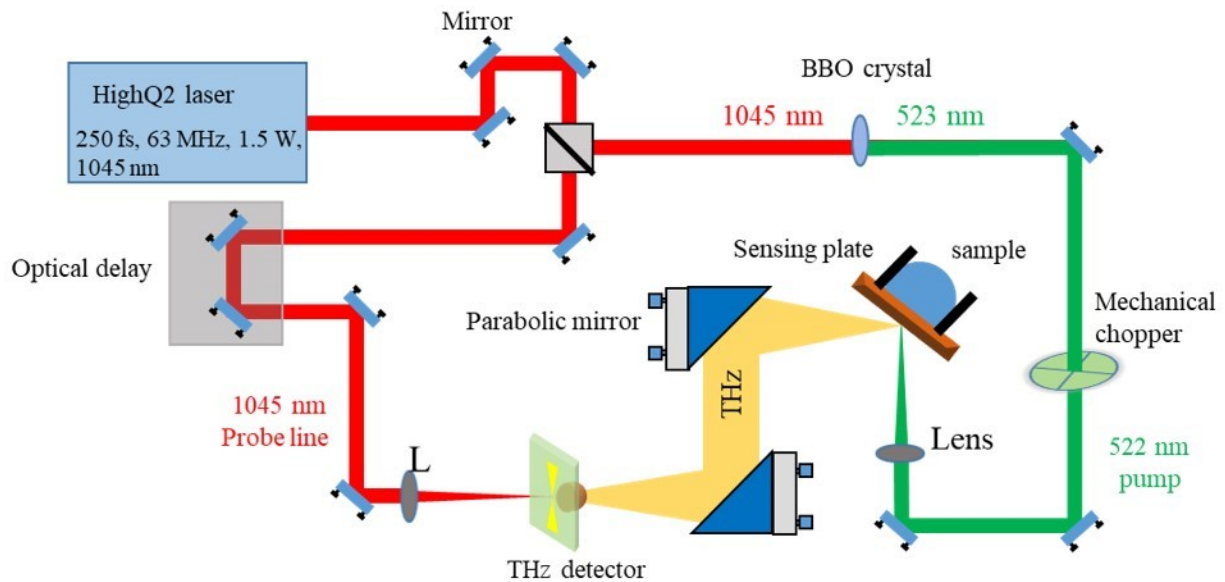


Figure S3. Optical setup of the TCM setup.

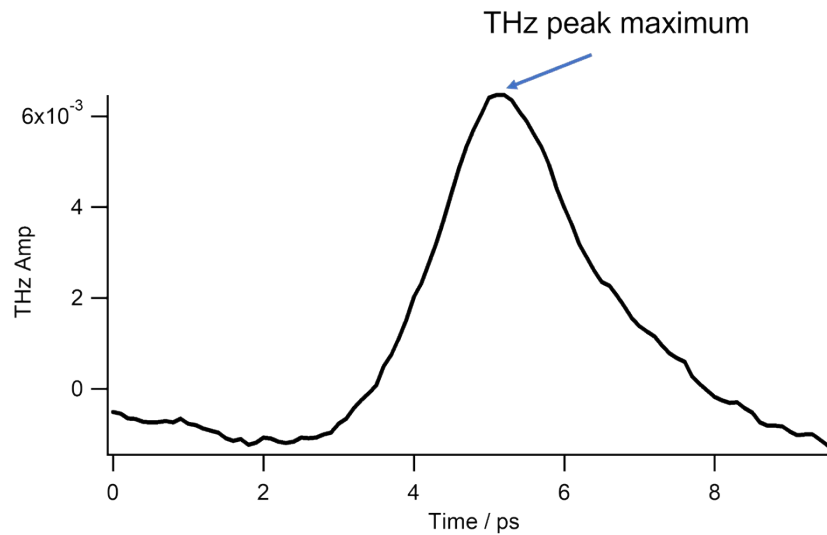


Figure S4: The THz waveform measured at the beginning of the TCM assay. The Time-delay stage is fixed at a time (5 ps) to scan the THz electric field peak in the x-y dimension.

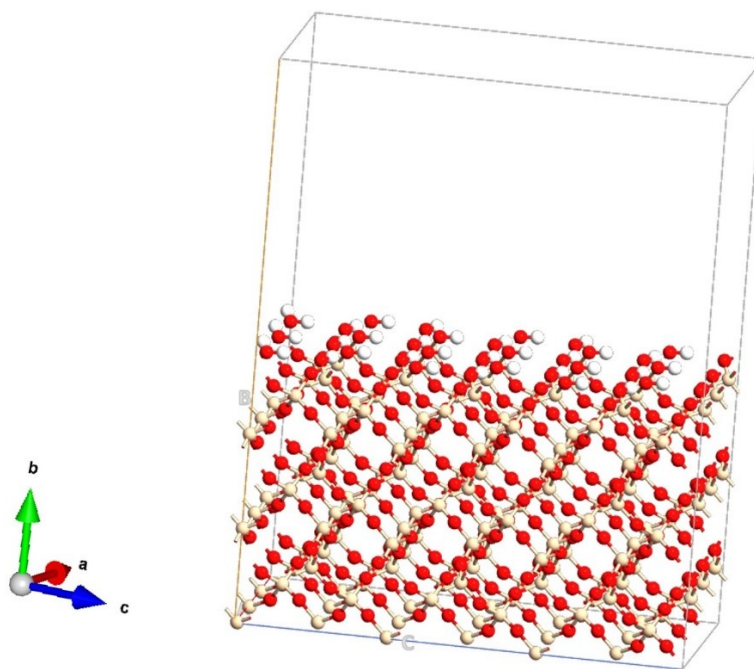


Figure S5. α -quartz surface. Color indication: red for oxygen, yellow for silicon, and white for hydrogen.

Preliminary optimizations:

In order to calculate the binding energy of AzPTES molecules on the surface of SiO₂, we need to calculate the minimum free energy of the atomic arrangements appearing in Eq. (7). We first optimized our model SiO₂ surface and AzPTES molecule.

We have considered the SiO₂ α -quartz structures. A DFT optimization at 0 K was performed to determine the optimal mesh parameters. These are, $a = 5.02 \text{ \AA}$, $b = 5.02 \text{ \AA}$ and $c = 5.51 \text{ \AA}$. Then a section was created following the direction (100) followed by lengthening the b axis to create a surface (fig. S4). The missing bonds in the oxygen atoms on the surface have been supplemented by hydrogen atoms. The new unit cell has been optimized to the following dimensions: $a = 5.02 \text{ \AA}$, $b = 22.11 \text{ \AA}$, $c = 8.70 \text{ \AA}$. In this work, we have used the simplified form of the AzPTES molecule shown in figure S5. In fact, the AzPTES molecule is made up of three ethyl groups bonded to oxygen atoms. We assumed that methyl groups do not participate in the adsorption reaction of AzPTES on the surface of SiO₂ and that the molecule shown in Figure S5 adsorbs to the surface by bonding its Si atom with an Si atom from the surface via a common oxygen atom. For this reason, we replaced the methyl groups by single H atoms. Our AzPTES model molecule has been optimized at 0 K to determine its minimal free energy.

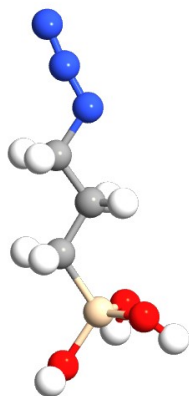


Figure S6. The simplified AzPTES molecule used in this work; gray: carbon, white: hydrogen, red: oxygen, yellow: silicon, blue: nitrogen

Identification of active sites:

Active sites have been identified at oxygen atoms on the surface capable of accepting hydrogens. The distinction between the sites was made on the basis of the hydrogen bonding energy to the surface in a unit cell since we consider that the entire surface will be covered with hydrogen. In this process, two types of non-equivalent oxygen sites were identified with relatively close hydrogen binding energy (-1.15 eV and -1.22 eV). Furthermore, the distance between these sites is of the order of 2.7 \AA (Figure S6). This distance is relatively small compared to the size of the

molecule AzPTES of figure S5 ($8.64 \text{ \AA} \times 2.66 \text{ \AA}$), which shows the impossibility of adsorbing two molecules on two close sites in the elementary cell.

In this work, a hydrogen atom from site number 1 was replaced by an AzPTES molecule. In this process, the AzPTES molecule loses one of its OH moiety while the surface loses an H atom, thus forming a water molecule according to the reaction



where $\text{SiO}_2 * \text{AzPTES}$ is the arrangement shown in figure S7 in which the Si atom of the model AzPTES molecule is bonded to an Si atom of the surface via a common oxygen atom.

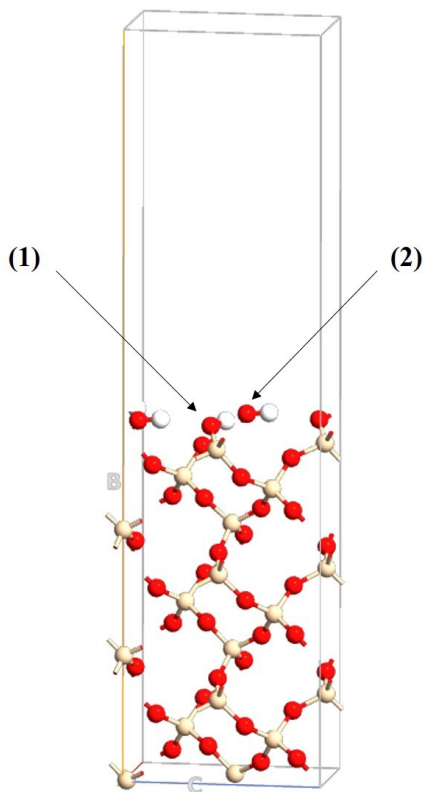


Figure S7. Potentially active sites in the unit cell of α -quartz.

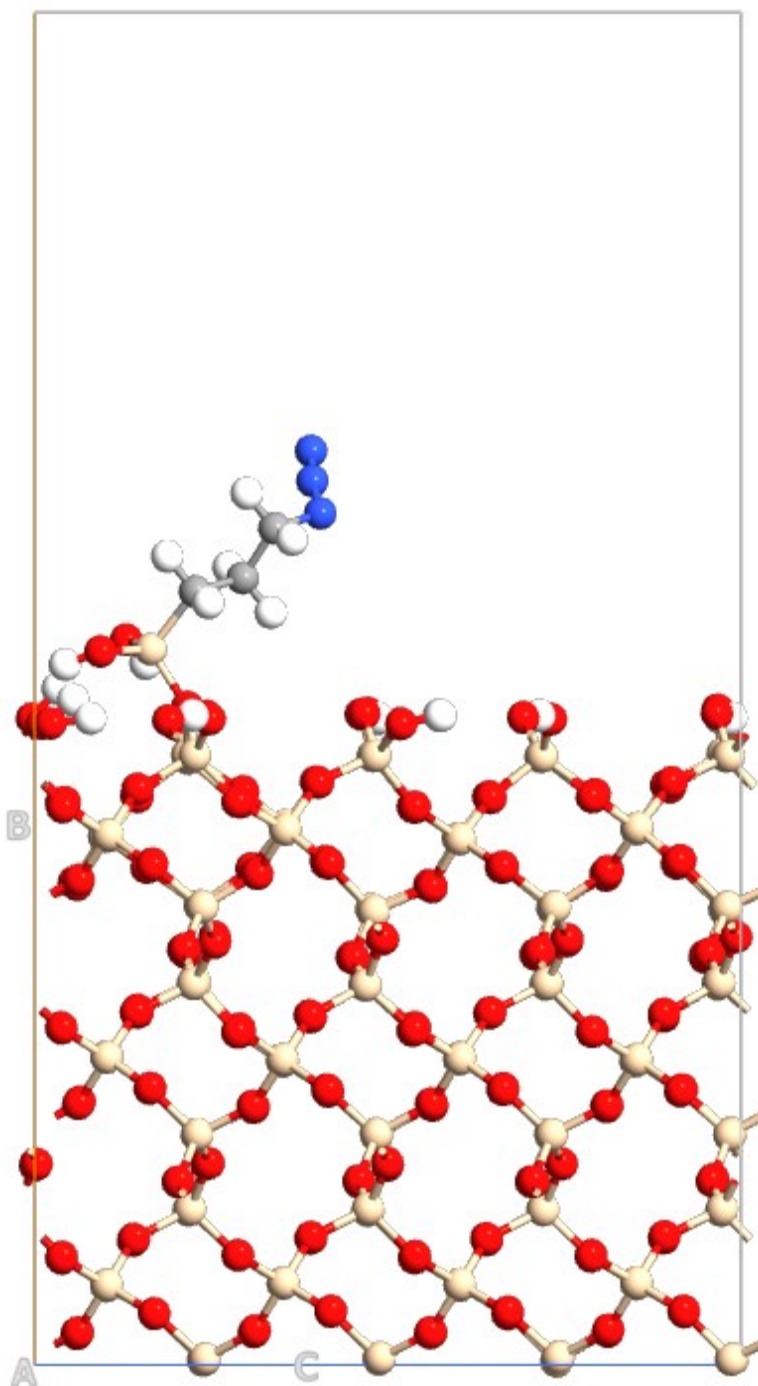


Figure S8. Adsorption of the molecule AzPTES on the surface of the 3x2x1 super cell.

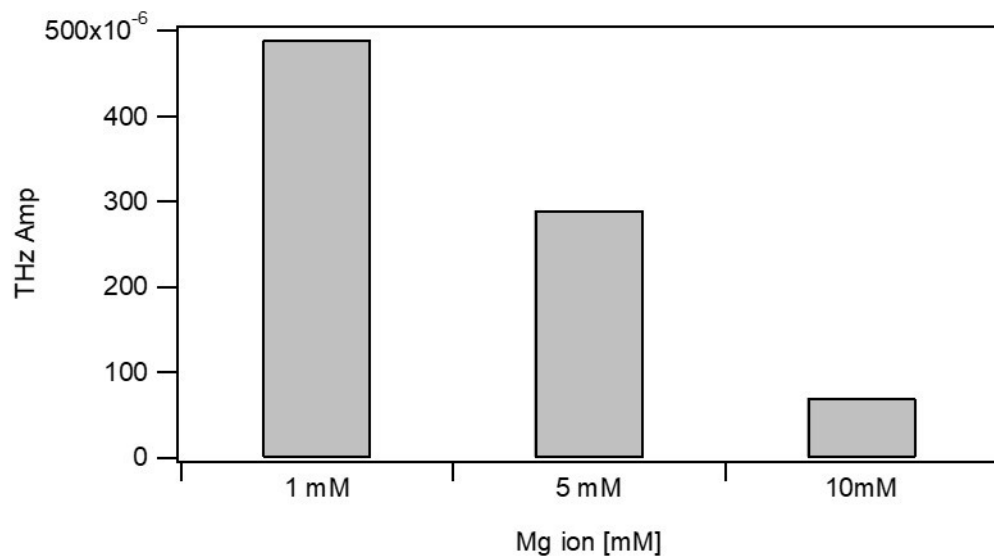


Figure S9. TCM response to 1 μM of kanamycin as a function of Mg^{2+} concentration.

Super-cell	Surface (\AA^2)	Number of AzPTES molecules / cm^2
1x1x1	43,674	2,2E14
2x1x1	87,435	1,1E14
2x1x2	172,257	5,8E14
3x1x1	131,196	7,6E14
3x1x2	262,5428	3,8E14
3x1x3	393,8896	2,5E14
4x1x1	174,957	5,7E+13
4x1x2	344,6854	2,9E14
4x1x1	525,2732	1,9E14
4x1x4	700,4313	1,4E14

Table S1. The number of AzPTES molecules / cm^2 for different geometries.