# Effect of Surface Facet on Iodine and Astatine Adsorption on Gold Nanoparticle

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The use of radioactive group 7 elements such as astatine (At) and iodine (I) labeled on gold (Au) nanoparticles are being researched as promising method for radiotherapy.[1,2)] Previous works have looked at their adsorption on a (111) surface and found that they are adsorbed covalently on the fcc hollow site.[3-5)]

The presence of edges in all gold nanoparticles mean that stepped surface should be considered as possible adsorption sites. We performed adsorption calculations on a stepped surface and found that both I and At are adsorbed on the edge sites stronger than the flat surface by around 0.2 eV. Based on this finding, we believe a more stepped surface may allow for better adsorption of the radionuclides intended for treatment use. Further details will be presented in the meeting.

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