Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Electronic structure and bonding of Au on SiO_2 cluster: A nano bullet for tumor QIANG SUN, QIAN WANG, PURU JENA, Virginia Commonwealth University — It is shown for the first time that gold atoms bind to silicon atoms with dangling bonds and serve as seeds for the growth of Au islands. The large electron affinity of gold causes significant change in the electronic structure of silica resulting in a substantial reduction in the HOMO-LUMO and the optical gap, thus allowing it to absorb near infrared radiation. This suggests that a small cluster can have similar functionality in the treatment of cancer as the large size nano-shell, but for a different mechanism. The advantage of having a small cluster with similar functionality as the large particle is that it can easily penetrate the crowded environments such as the biological milieu of cells and live tissues for effective drug delivery.

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Date submitted: 22 Nov 2004 Electronic form version 1.4