Metastability of a gold nano ring  QIAN WANG, QIANG SUN, PURU JENA, Virginia Commonwealth University — Due to the unique electronic, optical and catalytic properties, it is believed that gold nano-structures can have important applications in catalysis, molecular electronics, sensors, bioconjugate probes, gene mapping, and in the treatment of cancer and tumours. First principles calculations based on gradient corrected density functional theory show that a cluster of as few as 90 gold atoms can be stabilized in a ring structure having FCC(111) motif with the binding energy/atom and inter-atomic distance approaching 91% and 96% of the bulk values respectively. Although the ring structure lies 0.139eV/atom higher in energy than a poly-icosahedral structure, the calculated frequencies are real. Thus under appropriate experimental conditions it may still be possible to synthesize a metastable form of gold nano ring, as found in the recent experiment.