Defect states in monolayer transition metal dichalcogenides
MAHTAB KHAN, University of Central Florida — Monolayer transition metal
dichalcogenides (TMDC) have attracted considerable attention in the past few years.
They are direct bandgap semiconductors, with the conduction and valence band
edges at the doubly degenerate corners ($\pm$ K points) of the hexagonal Brillouin zone.
Recently, by using novel etching techniques, it was possible to remove a controlled
number of atoms from monolayer MoS_2, thereby creating a hexagonally shaped pit.
By solving the Dirac equation analytically, we show that a pit gives rise to bound
states with interesting properties. In particular, the optical selection rules turn out
to be very strict. We confirm our analytical results by means of numerical density
functional theory (DFT) calculations.

Mahtab Khan
University of Central Florida