



# Enhanced Pseudocapacitance of Low Energy Ion Irradiated Titanate Nanotube with Insight from Density Functional Theory Investigations



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### Experiments perform on Hydrogen Titanate Nanotube

- Hydrogen titanate ( $H_2Ti_3O_7$ ) nanotubes (HTNT) are grown on titanium foil by hydrothermal method.
- As prepared self-assembled and self-sustained hydrogen titanate nanotube arrays are irradiated with 5 keV  $Ar^+$  ion perpendicular to the substrate surface at  $1 \times 10^{16}$  ion/cm<sup>2</sup> and  $3 \times 10^{16}$  ion/cm<sup>2</sup> fluences using an ion-solid setup available at IIT Bhubaneswar

### Structural Analysis

Pristine

200 nm

Irradiated

200 nm

5keV  $Ar^+$

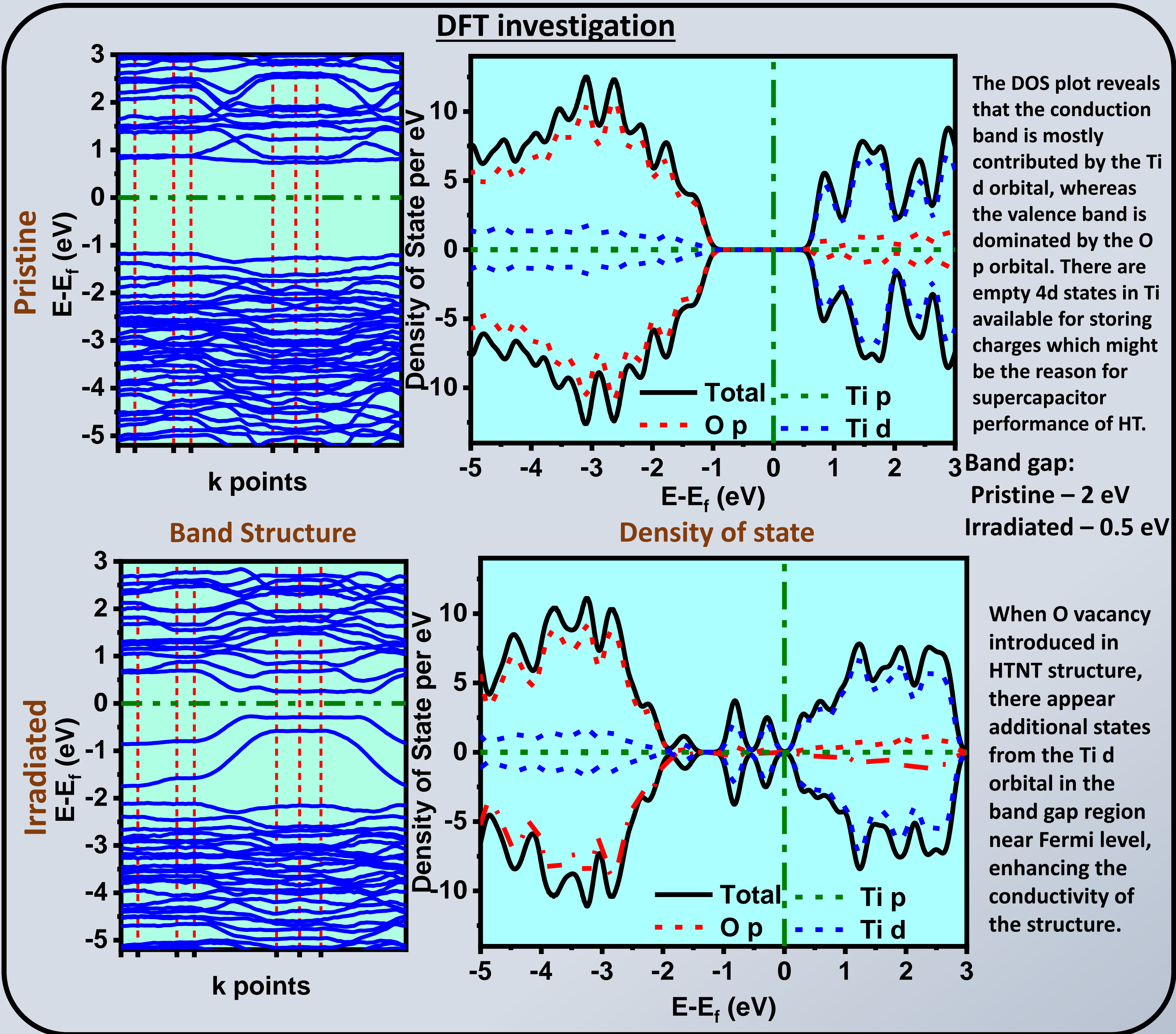
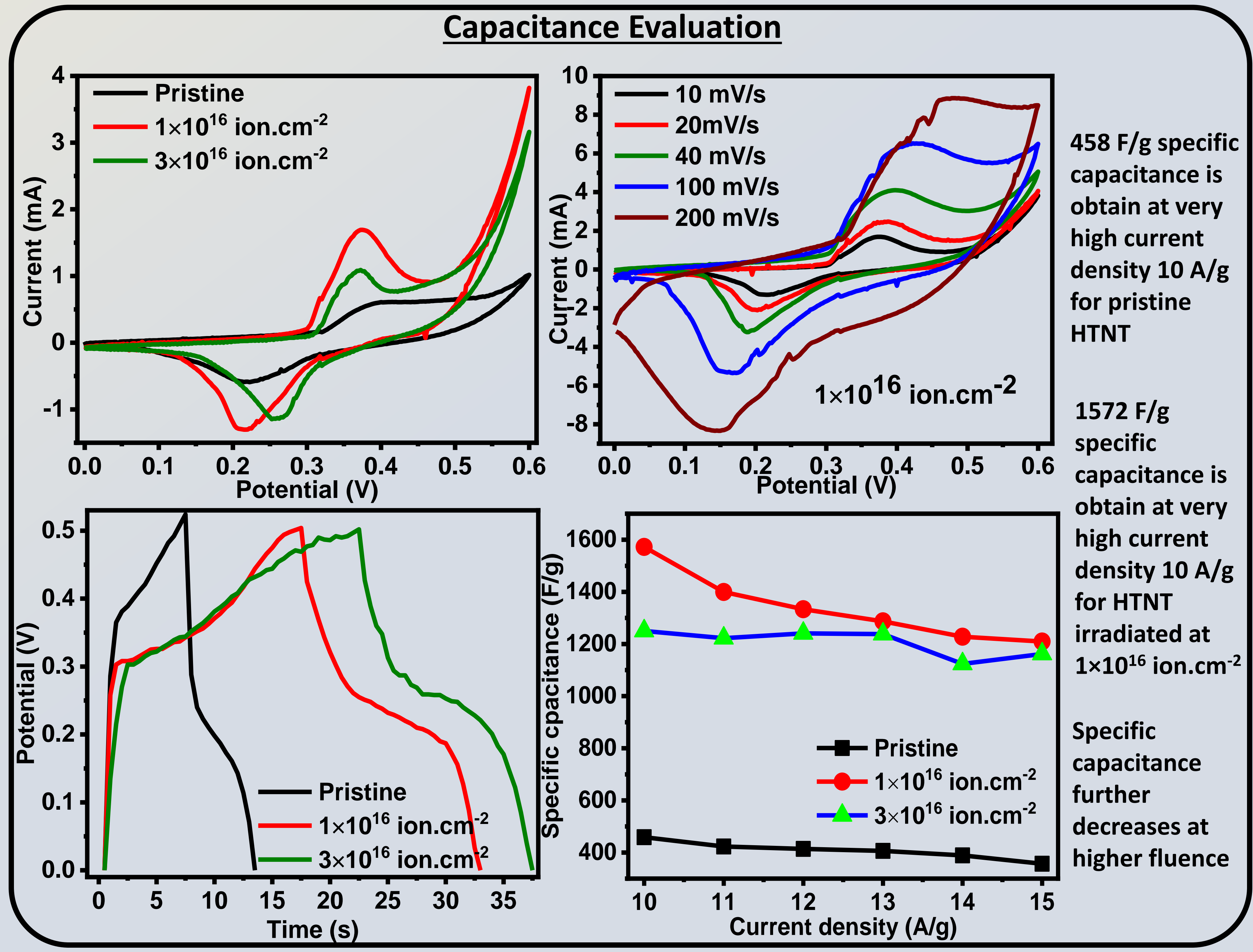
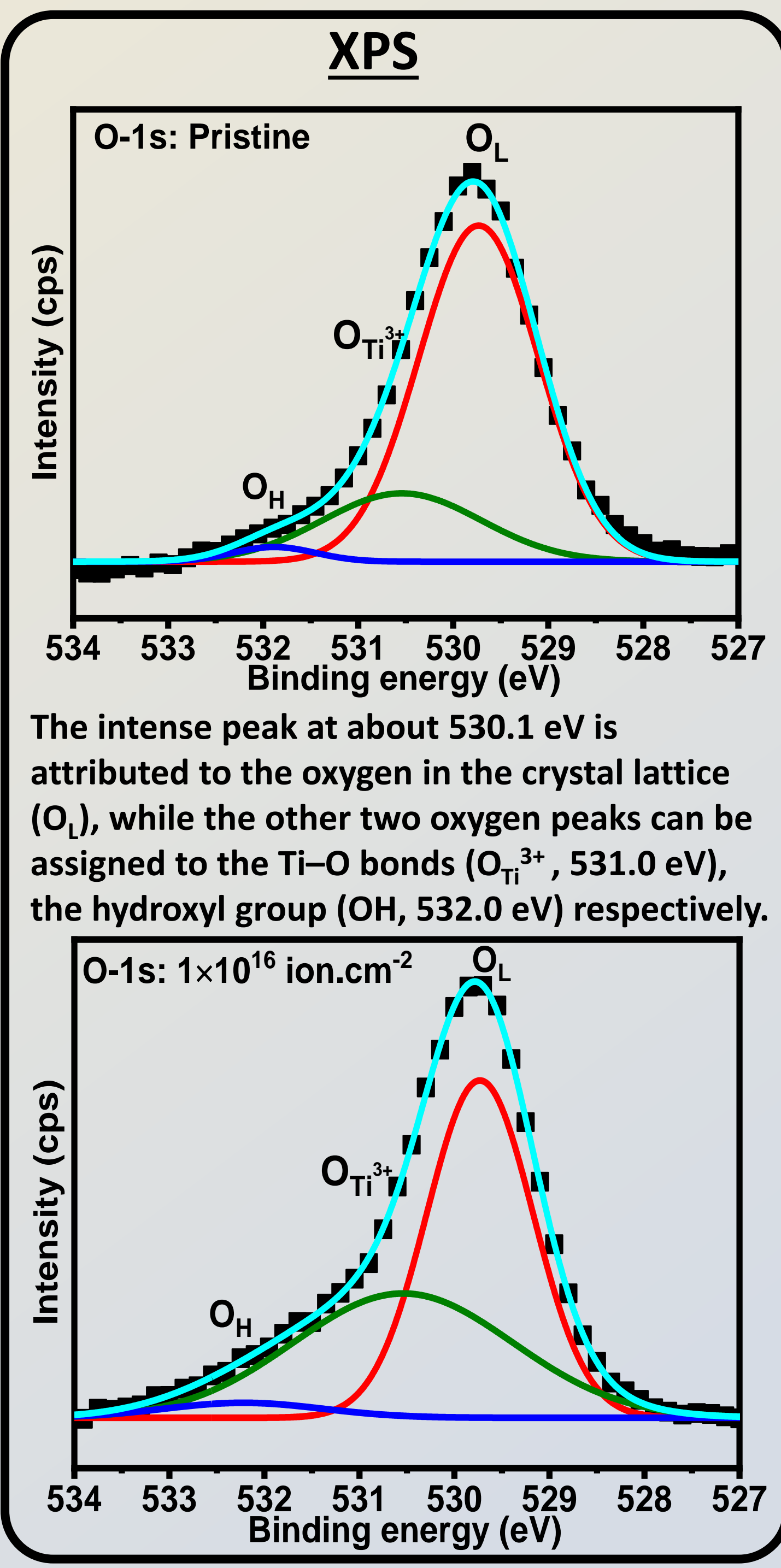
Mixed phase  $H_2Ti_3O_7$  and anatase  $TiO_2$  observed in both pristine and irradiated HT nanotube structures

### Welding Mechanism

Irradiated ion enter inside nanostructure and create internal defects (vacancy and interstitial) due to cascade collision. Some atom sputter out from the surface due secondary collision.

Recoil and sputter atom creates dangling bonds on the surface of the nanotubes. The amassed atoms in between two nanotubes bridge the gap by saturating the dangling bonds and establish a solid joining.

TRI3DYN Simulation



### Conclusions

- ✓ Self standing HT nanotube electrode is synthesised using hydrothermal method.
- ✓ Ion induced defect formation plays crucial role in nanotube surface modification.
- ✓ Welded network structure is modified controlling ion fluence.
- ✓ Mixed phase  $H_2Ti_3O_7$  and anatase  $TiO_2$  observed in both pristine and irradiated HT nanotube structures.
- ✓ HTNT transformation to titanium oxide due to defect induce recrystallization.
- ✓ Oxygen vacancy introduced into structure due to preferential sputtering, this increases conductivity of HT.
- ✓ At  $1 \times 10^{16}$  ion.cm<sup>-2</sup> fluence specific capacitance increases 4 time than pristine structure.
- ✓ Higher fluence, specific capacitance decreases due to less accessibility of pore in the network structure.

1. Pritam Das, M Rajbhar, Robert Glen Elliman, Wolfhard Moeller, Stefan Facsko, Shyamal Chatterjee, *Nanotechnology* 30 (2019) 365304.
2. Manoj K Rajbhar, Pritam Das, Biswarup Satpati, Wolfhard Moller, Stefan Facsko, Roman Bottger, Niranjana Ramgir, Shyamal Chatterjee, *Applied Surface Science* 478 (2019) 651.