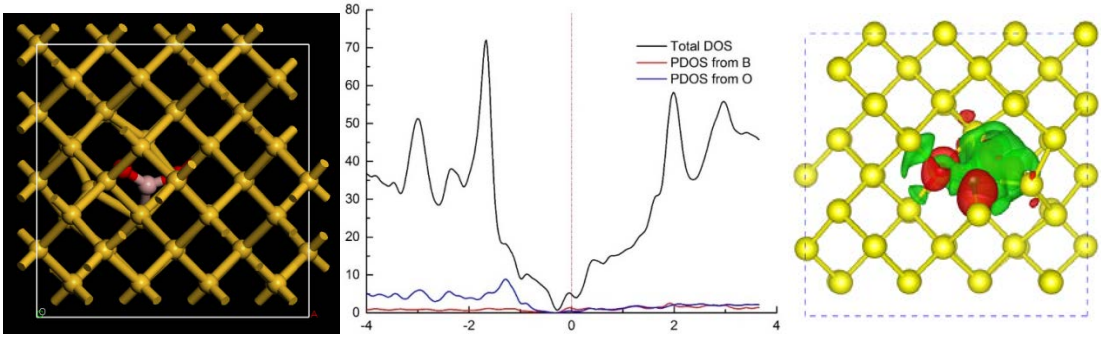
Modelling of Hydrogen Charge States and Defect Interactions for Crystalline Silicon

A recent break-through in the understanding and implementation of hydrogen passivation of crystalline silicon has been achieved at UNSW as part of its Government funded R&D program. Although originating from a project focusing on low cost, low quality silicon, the impressive results have subsequently lead to the application and demonstration of the advanced hydrogenation technology (AHT) to conventional commercial wafers, with similarly impressive results achieved. It is now recognized that the use of such techniques has the potential to raise open circuit voltage expectations for standard commercial p-type wafers from the present 650mV level to comfortably above 700mV, with corresponding improvements also in both the short circuit current density and fill factor. The net impact is that the long-term industry performance targets of 20% efficiency believed achievable with the standard commercial p-type wafers by 2020 are now believed to be way too conservative with production efficiencies in excess of 23% now being targeted by UNSW and its industry partners and well before this date.



Structure, density of states and electron redistribution after BO2 is introduced (both B and O are interstitial). The electronic distribution is defined as ρ_{tot}-ρ_{BO_2}-$\rho_{bulk\text{-}si}$, red: electron gain (mainly on O atoms); green: electron loss.

In order to further improve the understanding of hydrogen passivation, simulations based on first principles calculations and/or Molecule Simulation will be performed by Integrated Materials Design Centre (IMDC). We will model hydrogen passivation in crystalline silicon and its interaction with significant defects in silicon solar cells, thus shedding the light for the underlying mechanism and providing the possible way to improve efficiency. The work will focus on 1) what is the configuration of hydrogen in the silicon and the corresponding charge state; 2) how the defect and doping (B-O complex)

affect the performance of silicon as solar cells; 3)how excess carrier densities can affect these interactions and how stable passivation may be achieved.

The combination between experimental observations and theoretical explanation will give a clean and comprehensive picture for understanding the observed phenomena and expect to advance the silicon based solar cells.