

## **A COMBINED CLASSICAL MOLECULAR DYNAMICS SIMULATIONS AND AB INITIO CALCULATIONS APPROACH TO STUDY a-SI:H/c-SI INTERFACES**

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### **ABSTRACT**

In the silicon heterojunction solar cells, intrinsic hydrogenated amorphous silicon a-Si:H is used to passivate the crystal silicon c-Si surface to suppress the electrical losses at interfaces and to keep ultralow contact resistivity for the selective transport of one type of carrier only. We use ReaxFF (Reactive Force Field) molecular dynamics to efficiently simulate the thermalisation, quenching, and equilibration processes involving thousands of atoms forming realistic a-Si:H/c-Si interface structures. We generated snapshots of the equilibrated c-Si/a-Si:H interface atom configurations at room temperature. The ab initio characterization has been executed on selected configurations to monitor the electronic properties of the c-Si/a-Si:H interface. The evolution of the intragap states is monitored by analyzing density of states and charge density. This all will allow to design more efficient silicon solar cells belonging to the silicon heterojunction technology.

### **1 INTRODUCTION**

Passivation contacts is one of the most promising alternative techniques to crystalline silicon (c-Si) solar cells (SCs) for a high performance-to-cost ratio. An ideal passivation contact is able to suppress the electrical losses at interfaces and, at the same time, to keep ultralow contact resistivity for the transport of one type of carriers (holes or electrons) while hindering the transport of the other type.

In recent years, the silicon heterojunction (SHJ) solar cells reached the highest efficiency of 26.6% (Yoshikawa 2017), mainly due to the passivation contacts. In these devices, intrinsic hydrogenated amorphous silicon (a-Si:H) was used to passivate the Si surface and the p/n-type doped hydrogenated amorphous silicon was employed to select the transport carriers. Recently, it has been shown that hydrogenation of a-Si has beneficial effects in terms of reducing the overall strain energy of the a-Si network, with commensurate reduction of mid-gap states and orbital localization (Meidanshahi 2019).

The application of SHJs offers several advantages: first, a-Si:H provides efficient passivation of Si dangling bonds at the interface; second, field-effect passivation can produce a significant inversion effect at the a-Si:H/c-Si interface that is able to increase the carrier lifetime. Moreover, fewer process steps are required to build-up the SC, and the low-temperature (< 200 °C) processing allows the use of very thin wafers without any substrate damage.

The amorphous-crystalline heterointerfaces play a crucial role in the photovoltaic operation of SHJ technology, but the microscopic mechanisms of transport and recombination mechanisms at the interface are still poorly understood. The purpose of the present work is to simulate at atomistic resolution a large scale amorphous-crystalline heterointerfaces and to investigate the electronic properties (defects and

intragap states) that are preliminary to the study of the transport mechanisms underlying photovoltaic devices based on SHJ technology.

In order to design a predictive *ab initio* simulation of the a-Si:H/c-Si interface, it is essential to build up an atomic-scale model of the interface that exhibits the experimentally observed features and at the same time it is almost free of defects. Indeed, due to the limited number of atoms in an *ab initio* calculation, already few defects lead to a strong overestimation of the gap-state density, possibly even resulting in metallic behavior. An analogous study has been performed in a full *ab initio* approach by some of us (Czaja 2018a) for a smaller a-Si:H/c-Si interface formed by 336 atoms. A similar interface formed by 334 atoms was used to study the band offsets (Jarolimek 2017). In the present work, we combine ReaxFF (Reactive Force Field) molecular dynamics (MD) simulations and *ab initio* calculations to investigate the time evolution of the intra-gap states of an a-Si:H/c-Si interface structures constituted by 1,152 atoms. Therefore, we are considering a hetero-interface system larger than those of similar studies so that the periodic cell size effects are reduced. This allows us to model more realistic hetero-interfaces. The electronic structure is calculated and analyzed with a focus on the identification and characterization of the intragap states at the interface, which have a crucial impact on the device performance due to their role as recombination centers. Throughout the final thermalisation process, we monitor the evolution of the relevant structural and electronic properties, such as the defect distribution, the density of states and the potential barriers. In this way, insights are gained on how and why these properties change.

## 2 METHODS

We combined MD simulations using the ReaxFF training set parametrization and first principles calculations based on the density functional theory (DFT) to characterize the change of the electronic properties during the equilibration process. The high value of first principles calculations is to derive the physical properties directly from the basic interactions without introducing adjusting parameters.

The two a-Si:H/c-Si interfaces are made of hydrogenated amorphous silicon (a-Si:H) between two crystalline silicon (c-Si) slabs. The relaxed  $p(2\times 1)$  symmetric reconstruction of the Si(001) surface constitutes the c-Si side of the interface. It is formed by 576 Si atoms, 16 layers of silicon with 36 atoms each. The a-Si:H side of the system is generated by cutting the a-Si:H structure, built as in reference (Czaja 2018b), such that the surface area is equal to the c-Si side and the thickness is about 16 Å. It is composed of 512 Si atoms and 64 H atoms. The total length of the periodic cell is  $L_z = 46.44$  Å, while in the x- and y-direction the system has  $L_x = L_y = 23.22$  Å. Periodic boundary conditions are imposed in all directions.

The geometry of the *ab initio* relaxed structure is shown in Figure 1a: we use the PWscf (Plane-Wave Self-Consistent Field) code of the Quantum ESPRESSO suite (Giannozzi 2017; Giannozzi 2009) to relax the a-Si:H/c-Si system. Si and H ultrasoft pseudopotentials with Perdew-Burke-Ernzerhof (PBE) (Perdew 1996) approximant GGA exchange-correlation potential, available in the Quantum ESPRESSO library. The electronic wave functions were expanded in a plane-wave basis set with a kinetic energy cut-off equal to 40 Ry (the charge density cut-off was 240 Ry). The Brillouin zone integration for the self-consistent calculation is restricted to the  $\Gamma$ -point, which is justified by the sufficiently large super cell. Gaussian smearing of 0.08 Ry is needed to reach convergence due to defect states at the Fermi level. All the parameters are chosen by checking the convergence of the total energy of the system. The energy minimization is performed by using conjugate gradient (CG) minimization energy method, with the convergence threshold for self-consistency equal to  $10^{-6}$  Ry. Broyden-Fletcher-Goldfarb-Shanno (BFGS) quasi-newton algorithm is used to perform geometry optimization. Ionic relaxation is stopped when both the following conditions are satisfied: energy changes less than  $10^{-4}$  Ry between two consecutive self-consistent field (SCF) steps and all components of all forces were smaller than  $5 \times 10^{-4}$  Ry/Bohr. Then, this relaxed system is used as starting configuration for energy minimization and classical MD simulations.

A subsequent classical MD analysis of the final *ab initio* configuration has been carried out by means of LAMMPS (Plimpton 1995) using the ReaxFF training set parametrization previously employed for the

simulation of H bombardment of Si, Ge and SiGe (100) surfaces (Psofogiannakis 2016; Fogarty 2010). This training set parametrization includes the dissociation of Si-Si bonds in the Si<sub>2</sub>H<sub>6</sub> and Si<sub>2</sub>H<sub>4</sub> molecules, therefore taking into account for single and double silicon bonds, as well as Si-H bond dissociation of the SiH<sub>4</sub> molecule. The entire dissociation energy landscape is obtained by means of adiabatic energy DFT calculations vs. bond length and covers from the equilibrium distance to the dissociation limit. The energy dependence on valence and torsion angles in the Si-H force field is also incorporated. For example, for silicon bonds, the angular dependence is included in the form of the adiabatic DFT energy of the Si<sub>3</sub>H<sub>8</sub> molecule as a function of the Si-Si-Si bond angle, and torsional terms are adapted by including energy differences between chair, boat, and planar conformations of c-(SiH<sub>2</sub>)<sub>6</sub> six-member rings. Several other reactions are included, such as conversion of Si<sub>2</sub>H<sub>4</sub> to H<sub>3</sub>Si-SiH. Finally, the force field accurately take into account also the cohesive energy and the equation-of-state DFT predictions for various silicon crystal phases, including the simple cubic Si,  $\alpha$ -Si, and  $\beta$ -Si phases.

The complete MD analysis starts with T= 0 K minimization: firstly, fixing all cell dimensions: L<sub>x</sub>= L<sub>y</sub>= 23.22 Å and L<sub>z</sub>= 2·L<sub>x</sub> Å, then with L<sub>x</sub>= L<sub>y</sub> still fixed but with L<sub>z</sub> varying as an additional degree of freedom. The resulting geometry (see Figure 1b) is used as the initial condition for a subsequent quenching-thermalisation process. Initially, the system is heated up to 1100 K at zero pressure with a NPT (Nose-Hoover thermostat and barostat) (Hoover; 1996) for 325 ps and next it is cooled down to the desired final temperature of 300 K in 325 ps. In Figure 1c the final configuration of the quenching process is shown. A final thermalisation procedure is applied during 10 ns with 1 fs integration time step, keeping a constant temperature with a csld (Bussi 2007) thermostat to avoid the flying ice cube artifact. The pressure is controlled along the z coordinate exclusively, keeping L<sub>x</sub> and L<sub>y</sub> box sizes fixed and allowing L<sub>z</sub> to evolve isobarically (P= 0). Snapshots of the thermodynamic properties of the system as well as per atom dynamic values (coordinates, velocities, forces, etc.) are taken at 1 ps intervals for DFT DOS post-processing. The non-self-consistent calculation of the electronic states is performed on a 2×2×1 k-point grid, which was found to yield a sufficiently accurate representation of the relevant quantities (density of states, electron localization function, and charge density). In Figure 1d the configuration of the system at the end of the thermalisation process at 300 K is shown.

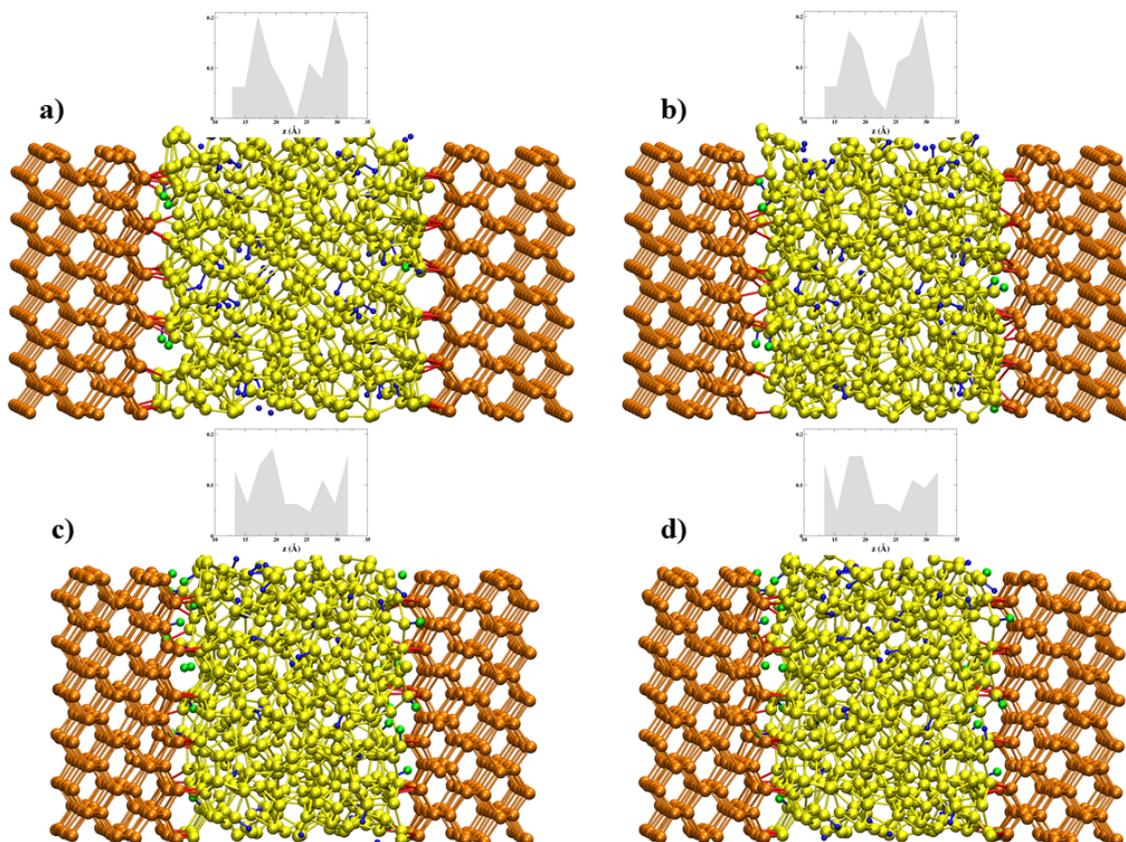


Figure 1: Snapshots of the a-Si:H/c-Si interfaces. a) The ab initio relaxed system; b) the system at the end of the minimization at  $T=0$  K; c) the system at the end of the quenching process; d) the system at the end of the thermalisation process at  $T=300$  K. The silicon atoms and their bonds are in orange in the c-Si side and are in yellow in the a-Si:H side, hydrogen atoms and bonds with silicon atoms are in blue. Bonds between c-Si and a-Si are in red. Moreover, the hydrogen atoms *close* to the interfaces (with a distance less than  $3.5$  Å to the c-Si sides) are in green. Above the configurations, the distribution of the hydrogen atoms along the  $z$  direction are reported.

### 3 RESULTS AND DISCUSSION

In this section, the results provided by the aforementioned simulations are reported. These results have been obtained using the CRESCO/ENEAGRID High Performance Computing infrastructure (Ponti 2014; Mariano 2019) where around 200,000 CPU hours have been used, and Piz-Daint/ACME clusters with 50,000 CPU hours..

In Figure 1 we report the snapshots of the c-Si/a-Si:H interfaces at different steps of the MD analysis. Silicon atoms and their bonds are in orange in the c-Si side and are in yellow in the a-Si:H side, hydrogen atoms and bonds with silicon atoms are in blue and bonds between c-Si and a-Si atoms are in red. It is applied a distance cut-off of  $2.85$  Å and  $1.7$  Å for Si-Si pairs and for Si-H pairs, respectively. In panel a) the ab initio relaxed system used as starting configuration of the MD simulations is shown. The following minimization at  $T=0$  K (see panel b) produces a shrinking of the simulation cell along the  $z$  direction, indeed  $L_z$  changes from  $46.44$  Å to  $40.67$  Å. This gives rise to a narrowing of the distance between c-Si and a-Si:H slabs. Then, in the quenching process, in which the system is heated up to  $1100$  K and cooled down to  $300$  K, it is observed a displacement of the hydrogen atoms toward the interfaces. To quantify this effect, we inspect the hydrogen atoms near to the c-Si side setting a distance threshold  $d_c=3.4$  Å (two times the distance cut-off for Si-H pairs). In Figure 1, the green atoms are hydrogen with distances to the

c-Si sides less than  $d_t$ . In the ab initio relaxed system there are 5 hydrogen atoms that increase to 7 at the end of the MD minimization at  $T = 0$  K. During the quenching, the hydrogen atoms move toward the interfaces increasing the number of green atoms up to 22. This value is also maintained in the following thermalisation at  $T= 300$  K. This effect is also highlighted in the graphs above each configuration, in which the distributions of the hydrogen atoms along the  $z$  direction are reported. In the first two distributions there are two peaks at about  $18 \text{ \AA}$  and  $30 \text{ \AA}$  and a well-defined minimum in the middle. On the contrary, in the last two graphs, it is observed a more uniform distributions: the two peaks are reduced to fill the empty space in the middle and to form new peaks at the borders in correspondence with the interfaces.

In Figure 2 we show the projected density of states (PDOS) of c-Si and a-Si:H ab initio relaxed, representing the PDOS of the a-Si:H/c-Si interfaces at  $T= 0$  K that will be used as comparison. We see that c-Si has a gap of around  $0.8 \text{ eV}$ , below the experimental value of  $1.1 \text{ eV}$  (Chiang 1989). It is well known that standard DFT (Perdew 1985) underestimates band gaps, due to the incomplete description of many-body effects. However, in this study the focus is on the formation of the intragap states related to the defects rather than on the evaluation of the band gap itself. From the PDOS in Figure 2b we see that broad peaks are induced from defects in a-Si:H bulk and at the interfaces.

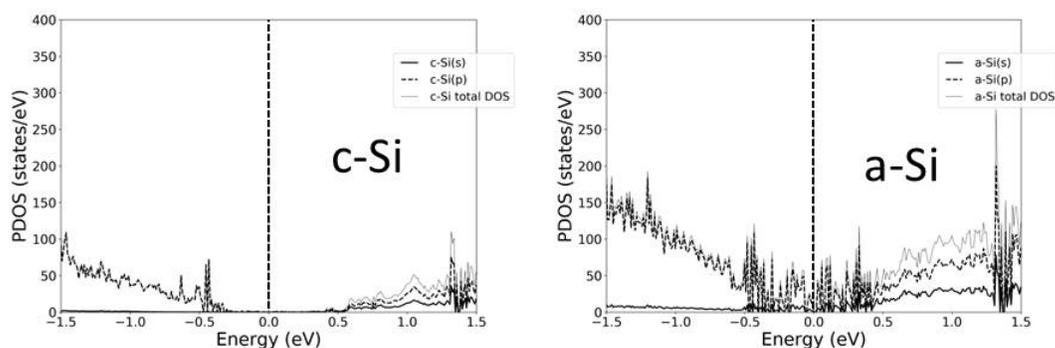


Figure 2: Projected density of states of crystalline and amorphous silicon of the ab initio relaxed a-Si:H/c-Si interfaces. The vertical dashed line at  $0 \text{ eV}$  evidences the Fermi energy.

We analyze the time evolution of the electronic properties of the a-Si:H/c-Si interfaces to monitor how intragap states change during the equilibration process at  $300 \text{ K}$  after the quenching. We follow the time evolution of the projected density of states (PDOS) during the equilibration process starting from  $t= 0 \text{ ns}$ , when the process begins until  $t=10 \text{ ns}$ . In Figures 3 and 4, the PDOS of c-Si and a-Si:H at  $t= 0, 1, 4,$  and  $10 \text{ ns}$  is shown, respectively. We observe at the start of the equilibration ( $t= 0 \text{ ns}$ ) that a dense concentration of peaks are found in the energy gap for the a-Si PDOS. Those peaks are related to defects at both the interface and in the a-Si:H bulk. In particular, one intense peak is found nearby the Fermi energy level at  $0 \text{ eV}$ . As the equilibration progresses, the energy of the PDOS peaks changes in energy and the corresponding intensity changes too, both in the intragap range and outside of it. Overall, after the ReaxFF MD annealing, quenching and equilibration we have a decrease of the density of the defects compared to that of the starting DFT relaxed a-Si:H/c-Si interfaces.

c-Si, T = 300 K

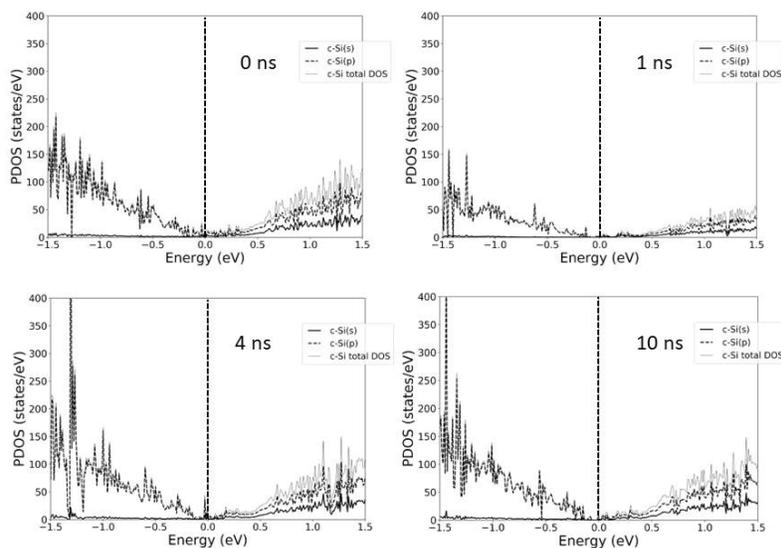


Figure 3: Projected density of states of crystalline silicon at 0, 1, 4 and 10 ns for T= 300 K. The vertical dashed line at 0 eV evidences the Fermi energy.

a-Si, T = 300 K

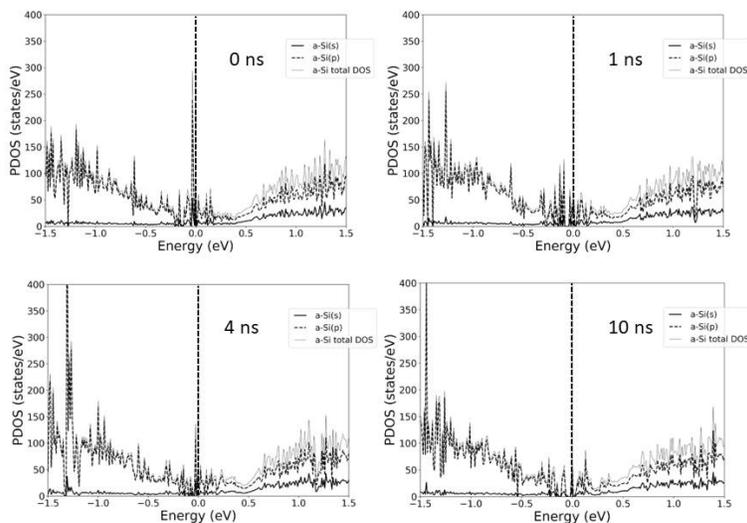


Figure 4: Projected density of states of amorphous silicon at 0, 1, 4 and 10 ns for T= 300 K. The vertical dashed line at 0 eV evidences the Fermi energy.

To gain a deeper understanding of the structural properties, a coordination analysis of the Si atoms is performed. A geometrical criterion is used to identify the nearest neighbors in the coordination analysis, applying a distance cutoff of 2.85 Å and 1.7 Å for Si-Si pairs and for Si-H pairs, respectively. Concerning the t= 10 ns snapshot, it is observed that the average number of neighbors of Si atoms is 4.01. In detail, 16

Si atoms have threefold coordination (1.4%), 1044 Si atoms have fourfold coordination (96.0%) and the remaining 28 Si atoms have fivefold coordination (2.6%). Just small variations have been found during the equilibration process taking into account that the average coordination number equals to 4.01 for the  $t = 10$  ns snapshot too. In conclusion, after the quenching process the system is quite ordered with a high percentage of fourfold coordinated Si atoms, and it keeps this condition during thermalisation at room temperature. By increasing the thermalisation temperature the number of fourfold coordinated Si has a monotonous increase until to 1054 atoms (96.9%) at 900 K.

In order to elucidate the spatial localization we calculated the local DOS (LDOS) of the intragap energy levels. In Figure 5, we compare the LDOS at  $t = 0$  and 10 ns. We found that defect states are localized both in the bulk of a-Si and at the a-Si:H/c-Si interface. Defects can be formed in the few c-Si layers nearest to a-Si:H. However, we see a change in the distribution of defects in the interval of time given to our simulation. Indeed the number and the intensity of the intragap states in the PDOS at the end of the equilibration process are lower than at the start. We investigated the coordination of the atoms nearby the LDOS isosurface at the interface indicated by the arrows in Figure 5. Following the above criteria for atomic distances, they are defects three-fold coordinated.

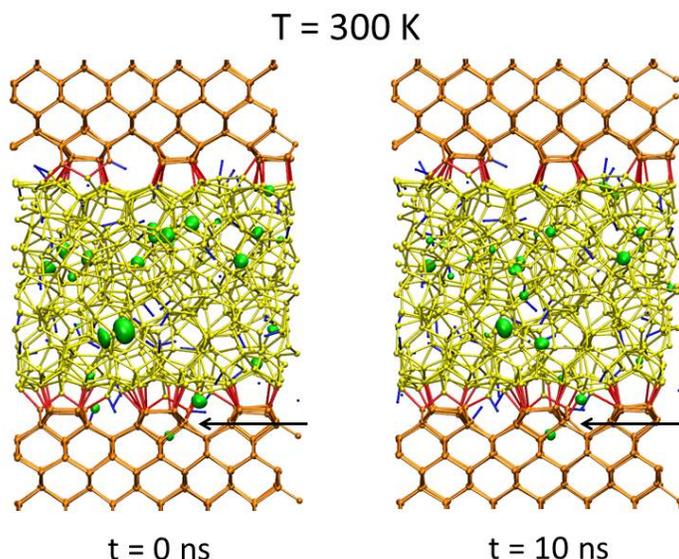


Figure 5: Local density of states of the intragap states of the a-Si:H/c-Si interfaces at the beginning a) and at the end b) of the thermalisation at  $T = 300$  K.

We calculated the energy potential averaged in cross section along the direction perpendicular to the interfaces, shown in Figure 6. The profile of the average potential has small variations along all the times of the simulation for 300 K. However, the energy barrier at the interface is almost the same for all the temperatures and times examined. We have investigated the charge transfer by calculating the difference of the charge density between the total system, and the c-Si and a-Si:H systems considered as isolated slabs, shown in Figure 7. We found that electron charge is accumulated along the c-Si/aSi:H interface and depleted from the nearby c-Si and a-Si:H surfaces. The two opposite pointing dipoles that are formed give rise to the potential profile showing an asymmetric barrier for electrons and holes, where the barrier for electrons (holes) is about 6.0 (2.5) eV. We average the potential over small (1.0 Å) and (5.0 Å) large spatial interval, so that the barrier is calculated as the difference between the local maximum (for electrons) or minimum (for holes) of the small interval average at the interface, and the large interval average in the middle of c-Si and a-Si:H bulk regions.

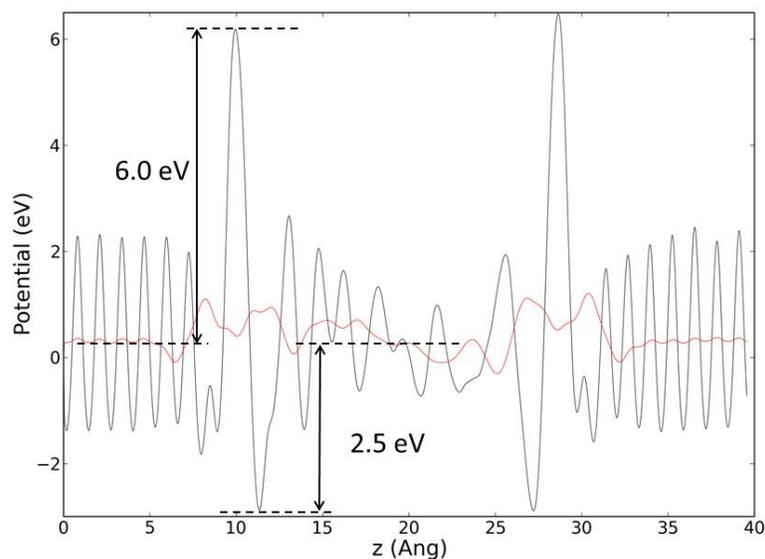


Figure 6: Energy potential averaged over the  $xy$ -plane at the end of the 300 K equilibration. The energy barriers at the interface are shown. The black (red) curve is the average over a spatial interval of 1.0 (5.0) Å.

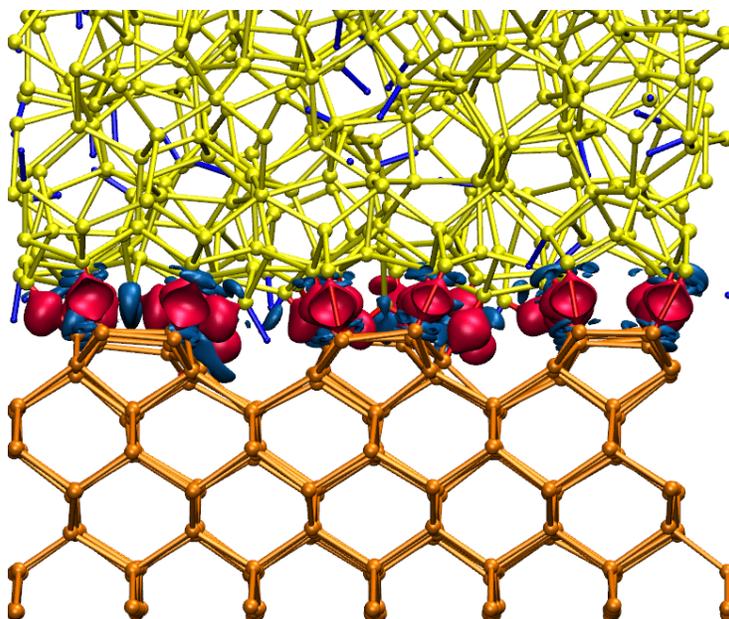


Figure 7: The  $c$ -Si/ $a$ -Si:H interface and the difference of the charge density between the total system and the  $c$ -Si and  $a$ -Si:H systems considered as isolated slabs at the end of the room temperature thermalisation. Red (blue) isosurface is the positive (negative) difference of the charge density.

## 4 CONCLUSIONS

In conclusion we combined ReaxFF MD simulations and ab initio calculations to investigate the time evolution of the intra-gap states of a large a-Si:H/c-Si interface system. Therefore, the electronic structure is calculated and analyzed with a focus on the identification and characterization of the intragap states, which have a crucial impact on the device performance due to their role as recombination centers. Throughout the annealing process, we monitor the evolution of the relevant structural and electronic properties.

An ab-initio relaxed system with a double a-Si:H/c-Si interface has been used as starting configuration for MD simulations. The minimization at  $T = 0$  K produces a shrinking of the system along the  $z$  direction of about 6 Å. Then, in the quenching process, in which the temperature raised up to 1100 K and cooled down to 300 K, it has been observed a displacement of hydrogen atoms towards the interfaces. This trend is maintained during the subsequent thermalisation at  $T = 300$  K for 10 ns, in fact, the concentration of hydrogen atoms near the interfaces remains almost constant.

We have found that at the end of the equilibration process of 10 ns at room temperature the intensity of the PDOS related to intragap states is decreased as well as the number of the electronic states into the gap. Nonetheless, the defects states are still localized both in the bulk of a-Si that at the interface with c-Si, until to be formed in the few c-Si layers nearest to a-Si:H. However, the system is quite ordered after the quenching process with a high percentage of fourfold coordinated Si atoms, and it keeps this condition during the final thermalisation. We found that electron charge is accumulated along the c-Si/aSi:H interface while it is depleted from the nearby c-Si and a-Si:H surfaces. The two opposite pointing dipoles that are formed give rise to different barriers to the each type of carriers favoring the hole transport while hindering the transport of electrons. Further studies are in progress to investigate the high temperatures effects on the electronic properties of realistic a-Si:H/c-Si interfaces. This study paves the way to the investigation of the transport mechanisms in order to design more efficient silicon solar cells based on the SHJ technology.

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