Polarization-Controlled Interface Charges for Generation of Open-Circuit Voltage Higher Than the Band Gap Towards "Polarization Photovoltaics" Solar Cell

Vishnukanthan Venkatachalapathy [1, 2], Lasse Vines [1], Andrej Kuznesov [1]

[1]Department of Physics, Centre for Materials Science and Nanotechnology, University of Oslo, Oslo, Norway

[2]Department of Materials Science, National Research Nuclear University "MEPhI", Moscow, Russian Federation

Email: vishnukanthan.venkatachalapathy@smn.uio.no

Abstract

Recently, solar cells have gained significant interest due to renewed attention to sustainability. The energy harvesting effectiveness of a solar cell centres are critically influenced by surface and interface properties inherent in the manufacturing of these devices. Conversion efficiencies over 40% have been achieved using conventional III–V semiconductor compounds as photovoltaic materials. The fundamental bandgap of the group III-nitride alloy system covers over a wider spectral region (from 0.64 to 6.2 eV) with tunable bandgap and strong absorption coefficient. However, bottleneck limiting the performance of such device arises from the potential barrier at the heterointerface due to the electron affinity difference. Another important factor is the existence of significant interface charges induced by spontaneous and piezoelectric polarizations due to non-centrosymmetric crystal structure. In turn, results in surface band bending depending on the interaction with surrounding atmosphere. Heterojunction (HJ) between n-ZnO and p-Si has a potential to perform as efficient and inexpensive solar cell. However, the relation between the polarization bound charges and the electronic properties of the HJ interfaces is not yet well understood. Calculated work function, φZnO (or barrier height) for ZnO varied from 5.02 to 0.33 eV as a function of Zn/O molar ratios. Surprisingly, a non-centrosymmetric crystal structure can develop a giant photovoltage. Specifically, the electron processes: photo-excitation, scattering, and relaxation occur with different probabilities. Considering, a hetero-structure with cubic and non-centrosymmetric material, each non-centrosymmetric layer can act as a photovoltaic, so that the overall open-circuit voltage across the multi-junction is large, potentially much larger than the bandgap. Fundamental issues considering wurtzite-GaN/cubic GaN and wurtzite-ZnO/cubic-CdO hetero-structures will be discussed towards next-generation solar cells.