Theoretical investigation of perovskite heterostructure interfaces

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Abstract

Due to a number of interesting properties, like feroelectricity, feromagnetism, and even multiferoism, perovskites have been attracting attention for over a decade, especially for solar cell applications. First attempts to make use of perovskites for photovoltaic applications did see some improvements in photovoltaic efficiency. However, the most prominent perovskite for photovoltaic applications, methyl ammonium lead iodide (MAPI), is not appropriate for large scale manufacturing and use, since it is composed from lead, in amongst other elements. Another reason that first attempts for production of perovskite solar cells failed was that MAPI is quite a bit unstable, as it can retain its properties for just a few minutes. Since then, a lot of improvements have been made, and there has been a lot of research in vast variety of other perovskites.

With a huge step up in computer technology, and with advancements in theoretical analysis of such systems, heterostructures became increasingly more interesting for research. By joining two materials together, a number of interesting properties can emerge at their interface. An example is absorber-buffer layer interface in photovoltaic cells. Newly obtained interface properties can be predicted by using density functional theory (DFT). With the use of DFT, one can dive into analysing the hetero-interface and look at what is happening with materials as they are joined into the heterostructure. By looking at the total potential energy at the interface, and comparing it to the total potential energy of slab structures of individual materials, one can obtain useful information about charge dynamics at the interface. Of large interest are either band offset at the semiconductor - semiconductor interface, or Shotky barrier at metal - semiconductor interface. Other useful information can also be obtained, like charge transfer at the interface, effective mass, charge polarisation, charge mobility, etc.

In this seminar, we will look into use of density functional theory in predicting heterostructure properties. DFT can be a useful tool in modelling a vast variety of heterostructures that can help overcome the shortcomings that the materials individually possess.

Keywords: DFT, heterostructure, interface, perovskite, photovoltaics

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