

Current Physical Chemistry

Special Issue on

Interfacial properties at the atomic/molecular level: from experiments, theory to simulations

Call for Paper

Aims and Scopes:

Interfacial properties such as interfacial forces, morphologies, surface energy are central to the performance of different devices or various composites. Especially, with the developments of fabrication technology and analytical techniques, the size of devices or building blocks has narrowed down to the nanoscale, molecular or even atomic level. The control of the interactions between the interfaces becomes critical to the device performance or materials properties, which involves a variety of research fields ranging from the tradition polymer composites to the research hotpot solar cells, fuel cells, etc. For example, the engineering of the interface between donor and acceptor in bulk heterogeneous junction solar cells can significantly affect the charge carrier injection, transfer, collection and finally the power conversion efficiency of solar cells. More obviously, the design of the interface between nanofillers and polymer matrix is of paramount importance to the mechanical and thermal properties of composites, such as Young's modulus, fracture toughness, glass transition temperature, etc. Although progress has

been made to the understanding of the interface properties, nonetheless accurate and delicate molecular design at the atomic level requires deeper insights into the fundamental mechanisms of the interface. Therefore, efforts from experimental, theoretical or simulation works are urgently needed to tackle the poorly understood relationship between atomic interface and macroscopic properties in order to underscore people's capability of better engineering.

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