

The macroscopic vs. the atomistic view of surfaces

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The macroscopic and experimental view of surfaces and definition of surface properties often differs from the atomistic view. As an example one can cite the classical view of the electrical double layer around colloidal particles, where a smooth flat surface is assumed to be in contact with pointwise charges in a continuous media. When looking at atomistic simulations, one generally sees clear density variations and the ions have a finite size. How to deal with these differences when comparing atomistic models to often macroscopic experimental measurements? These questions will be the topic of the talk and are discussed on a few examples (colloidal systems, porous materials ...). Some general guidelines and strategies to increase the consistency between macroscopic experimental and atomistic theoretical results obtained at different length scales are outlined.