Ab Initio Simulations of Interfaces between Liquid Metals and Solids

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The understanding of the properties of liquid metals in contact with a solid wall is of both physical and technological interest, involving processes such as soldering, lubrication, wetting or crystal growth. The theoretical study of these properties requires a correct description of the forces acting between the atoms within the liquid, between the atoms within the solid and between solid and liquid atoms. Even if models can be set up for the first two types of interaction, the modelling of the interfacial forces is in general subject to important difficulties. This is where ab initio calculations take a most important role.

On the other hand liquid systems and in particular liquid surfaces require large simulation cells due to the lack of periodicity, and this need is not easily met by standard ab initio simulation methods.

In this talk we offer some examples of the use of the so called "orbital free" ab initio simulations [1] in the study of liquid metals on solid metals, including model systems (atoms pinned to their ideal positions in the solid) as well as realistic metallic solids. The absence of orbitals in the formulation enables the use of thousands of atoms in the study through long simulation times.

For non-metallic solids different techniques have to be considered, and we show here some preliminary results for the simulation of a liquid metal on a semiconducting surface, using an ab initio method (PARSEC) which is amenable to a very efficient paralellization, based on a treatment in real space of the electronic structure part of the problem [2].

References

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