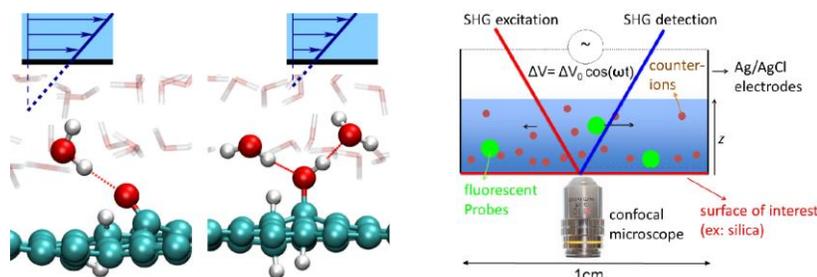


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Nanofluidic energy conversion using reactive surfaces



Water desalination and sustainable energy harvesting are among the greatest challenges of our society, and nanofluidics offers promising solutions to address them. Nanofluidic energy conversion systems rely on electrokinetic (EK) effects, which couple different types of transport (hydrodynamic, electric, ionic, thermal...) at interfaces. EK effects are sensitive to the molecular detail of interfaces, and should thus depend on their physical chemistry. Yet the possibility to couple surface reactivity and EK transport to enhance the performance of nanofluidic devices has never been studied to the best of our knowledge.

In this project, we explore these couplings in order to design innovative nanofluidic systems for sustainable energies, focusing on waste heat harvesting. To that aim, we gather experimentalists and theoreticians who work on the same systems, and who probe simultaneously the physical chemistry of the interfaces as well as their transport properties, combining *ab initio* and force field molecular dynamics simulations, non-linear optics, and macroscopic transport measurements. This strategy opens the way to find optimal situations where reactive interfaces have a large impact on nanofluidic energy conversion.

We are looking for a master student to participate in the numerical part of this project. In particular, the student could work on one of these subjects:

- exploring the transport properties of reactive water-oxide interfaces with *ab initio* molecular dynamics;
- developing fast and reliable methods to measure friction and heat transfer at liquid-solid interfaces;
- predicting the efficiency of electrokinetic energy conversion at hydrophobic surfaces with mobile charges.

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